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On the 1D Coulomb Klein–Gordon equation

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Abstract
For a single particle of mass m experiencing the potential $-\alpha/|x|$, the 1D Klein–Gordon equation is mathematically underdefined even when $\alpha \ll 1$: unique solutions require some physically motivated prescription for handling the singularity at the origin. The procedure appropriate in most cases is to soften the singularity by means of a cutoff. Here we study the bound states of spin-zero particles in the potential $-\alpha/(|x| + R)$, extending the nonrelativistic results of Loudon (1959 *Am. J. Phys.* **27** 649) to allow for relativistic effects, which become appreciable and eventually dominant for small enough mR: they are totally different from conclusions based hitherto on mathematically simple-seeming matching conditions on the wavefunction at $x = 0$. For realizable R, all relativistic effects remain very small; but with mR decreasing to order α^2 the ground-state energy E decreases through zero, and soon after that mR reaches a finite critical value below which E becomes complex, signalling a breakdown of the single-particle theory. At this critical point of the curve $E(mR)$ the Klein–Gordon norm changes sign: the curve has a lower branch describing a bound *anti*particle state, with positive energy $-E$, which exists for mR between the critical and some higher value where E reaches $-m$. Though apparently unanticipated in this context, similar scenarios are in fact familiar for strong short-range potentials (1D or 3D), and also for strong 3D Coulomb potentials with α of order unity.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction and conclusions

1.1. Background and motivation

Ah! What avails the classic bent

and what the cultured word,

before the undoctored incident

that actually occurred?

The hydrogenic potential $-\alpha/r$ in spaces with other than three dimensions continues to supply quantum mechanics with entertaining problems which are by no means exhausted. In 1D, the question is complicated by the fact that wave equations featuring $-\alpha/|x|$ are mathematically underdetermined, making it necessary either (i) to supplement them with matching conditions at the origin, or (ii) to introduce a cutoff to soften the singularity there. For definiteness, we shall consider a single particle of mass m in the nominally weak potential

$$V(x) = -\alpha/(|x| + R), \qquad \alpha \ll 1, \quad mR \ll 1, \tag{1.1}$$

near but not in the limit where $mR \to 0$. We use natural units $\hbar = 1 = c$.

We aim to explore cutoffs handled relativistically, but in order to see cutoffs in context must start with some comments on the recently more popular approach (i). Physically speaking, the role of the supplementary matching or boundary conditions in this approach is to select a Hilbert space where the underlying Hamiltonian and the momentum operator $-\mathrm{i}\partial/\partial x$ are self-adjoint. The problem is essentially the same as one faces in 3D for potentials singular like $1/r^n$, with $n \geqslant 2$: it turns on ideas readily legible from a remarkable early paper by Case (1950), plus the comments on it by Popov (1971b, section 4). The mathematical difficulties stem from the fact that the operators in question are not (even) essentially self-adjoint, i.e. that their self-adjoint extensions[1] are not unique. For the requisite 1D Schrödinger equation, this is spelled out in modern terms e.g. by Fischer *et al* (1995) and by Tsutsui *et al* (2003), who make it very clear that the matching conditions must be chosen to reflect the physics governing the particle near the origin. But many papers, while acknowledging this requirement at some point, nevertheless adopt conditions that appear to be motivated purely by notions of mathematical simplicity, and then proceed to formulate the consequences in unguarded language suggesting, or allowing the reader to infer, that they apply to any physical 1D model one might reasonably be interested in. Examples include the otherwise illuminating discussions by Moshinsky (1993), plus the related exchange between Newton (1994) and Moshinsky (1994); by Kurasov (1996), plus the related exchange between Fischer *et al* (1997) and Kurasov (1997); and by Gordeyev and Chhajlany (1997).

Often the purpose seems to be the elimination of those roots of the indicial equation that yield radial wavefunctions supposedly too singular[2] at the origin. But in most applications the potential itself is not truly singular there. It is smoothed already in the 3D hydrogen atom (by the finite charge density of the proton), and also in at least two important examples where 1D serves to model a well-understood limit of or to approximate a 3D system: namely hydrogen-like atoms in very strong magnetic fields (where the electron is effectively threaded

[1] For a sketch of the theory of such extensions see e.g. Galindo and Pascal (1990), and for a fuller account Reed and Simon (1980, 1975). Thaller (1992) discusses the relatively straightforward and uncontroversial applications to the 3D potential $-\alpha/|r|$, where, fortunately, the extension required by the Dirac equation is unique.

[2] As emphasized by Armstrong and Power (1963), amplifying Dirac (1947), the simplest pertinent observation in 3D is that ∇^2 acting on functions that diverge like $1/r$ produces a delta-function $\delta(\mathbf{r})$ absent from the true equation. But this argument fails in 2D and 1D. Some singular 1D solutions appear in appendix E below.

on a finite-radius cylinder surrounding a field line: see e.g. Ruder *et al* 1994); and an electron confined to the surface of a nanotube in the presence of an ion (see e.g. Bányai *et al* 1987). In such cases the present writer can attach physical significance only to potentials like (1.1) smoothed by a cutoff; and, by courtesy, to systems with arbitrarily small but still finite mR. Many other examples occur in other papers easily found through their citing the seminal work of Loudon (1959); and López-Castillo and de Oliveira (2006) make some interesting general remarks about ways that 3D physics can generate 1D problems.

Unfortunately, in 1D, unlike 3D, the prescriptions widely favoured by recent papers applying method (i) to the unsmoothed potential $-\alpha/|x|$ yield spectra quite different from what one finds when smoothing is just about to disappear. The one important case where there is no conflict is murium, a charged particle bound by image forces to a half-space it cannot penetrate, so that the wavefunction must vanish on the surface: say an electron above liquid helium (e.g. Nieto 2000). By contrast, Andrews (1976, 1988) argues that the singularity by itself acts like an impenetrable barrier, turning particles on the half-lines $x \gtrless 0$ into mutually disjoint systems, and parity into an empty concept: a suggestion that the more complete discussions already cited indeed show to be compatible with prima facie quite plausible matching conditions, though it is not generally helpful for guiding calculations with finite cutoffs. But, uniquely, Andrews does comment on cutoffs to the extent of spelling out that short of the limit they admit tunnelling at finite rates, with consequent level splittings in the observed spectra.

The literature cited so far relates to the Schrödinger equation, which, using cutoffs, i.e. by method (ii), was solved half a century ago by Loudon (1959). His results are summarized in appendix A: there are levels with $E_n \simeq m-\alpha^2 m/2n^2$, $n = 1, 2, 3, \ldots$, each a near-degenerate parity doublet with even *above* odd; plus a nondegenerate even-parity ground state with an energy conveniently written as $E_0 = m - \alpha^2 m/2\xi^2$. As R vanishes, the degeneracies become exact, while E_0 diverges because $1/\xi$ diverges, roughly like $|2\log(\alpha m R)|$.

The present paper considers the corresponding 1D Klein–Gordon (KG) equation for relativistic spin-zero particles. Though it will turn out that, for these, the relativistic effects peculiar to 1D are largely academic (cf appendix A), they do bear on interesting questions of principle. The mathematics governing singular potentials in 1D are the same for the KG as for the Schrödinger equation. In particular, one faces the same choice between approaches (i) and (ii); but the existing literature is scanty, and far less systematic. Following variants of method (i), i.e. as consequences of the singular potential $-\alpha/|x|$, the first paper, by Spector and Lee (1985), noted the possibility of a tightly bound (even-parity) ground state with total energy $\tilde{E}_0 \equiv m[1/2 - \sqrt{1/4-\alpha^2}]^{1/2} \simeq \alpha m$, which nowadays might be called a hydrino (cf Dombey 2006); Moss (1987) rejects this; and de Castro (2005) claims that there are no even-parity bound states at all. Other papers can be traced through references given by these[3].

To guard the reader against false expectations, it may be worth repeating that we are not concerned with the mathematical problems attending the truly singular potential $-\alpha/|x|$. We study only the physical problem of the potential (1.1) with finite R, whose mathematics are unambiguous: the limit $mR \to 0$, though it may be interesting, is regarded as secondary. The writer's view is that, sadly, one has to live with the fact that the mathematical options available at present for $-\alpha/|x|$ cannot adequately elucidate the physics of $V(x)$.

[3] The 3D KG equation and the technically similar 2D Dirac equation have been discussed recently by Dombey (2006). Still to be explored are the implications of method (ii) for the challenging cases of the 2D KG and the 1D Dirac equations, which suffer from the additional difficulty that the roots of their indicial equations are complex. Experience has taught the writer to make no guesses about what such studies might reveal. A paper on the 1D Dirac equation by Benvegnù (1997), not citing Loudon's work, uses method (i), and (as one would expect) identifies no relativistic generalization of the level E_0.

1.2. Preview and summary

As just explained, we have nothing new to say about the singular potential $-\alpha/|x|$ tackled directly (but cf appendix E); instead, we adopt (1.1) and follow method (ii) by applying Loudons's ideas relativistically. The differences from method (i) are drastic[4]. (a) Under appropriate conditions (mR small but not too small) the consequences of the KG equation must reduce to those of the Schrödinger equation, and prescriptions under which they do not can have no application. (b) A ground state with relativistically strong binding does eventually evolve from Loudon's E_0, but it is not truly related to the state with energy $\tilde{E}_0$ noted by Spector and Lee. (c) Finally, what happens (or rather would happen) at unrealistically small $mR \sim \mathcal{O}(\alpha^2)$ is unlike anything yet envisaged under method (i), being governed by a breakdown of single-particle theory explored hitherto only *à propos* of strong short-range potentials, and of Coulomb potentials with α of order unity rather than small.

Sections 2.1, 2.2 write down the wave equation, defining scaled parameters and variables essential to make it manageable: in particular, $\delta \simeq \alpha^2$ from (2.13), (2.14) measures the strength or rather the weakness of the potential; λ or $\beta \equiv \lambda/\delta$ from (2.7), (2.15) measure the eigenvalue $E \equiv \hbar\omega$; and Z or $s \equiv mR/\delta$ from (2.8), (2.15) measure the cutoff. Section 2.3 identifies solutions f integrable to infinity, and their slopes, equations (2.24)–(2.28), in terms of standard confluent hypergeometrics. Section 3 then finds an eigenvalue equation for E by subjecting f to the boundary conditions at the origin, appropriately to the parity. Section 4 uses these results to show that the levels subdivide naturally into *Balmer-like* and *anomalous* states. We define Balmer-like states as those bound lightly, i.e. nonrelativistically: the name is chosen by hindsight, since (for all $mR \leqslant \mathcal{O}(1)$) their energies turn out to be very close to those given by the Balmer formula for ordinary (3D) hydrogen, conformably to Loudon's results already quoted in section 1.1. Section 5 works out some details as mR shrinks, showing in particular how the splitting of the parity doublets depends on n. Any other state is defined to be anomalous; in fact it will turn out that there is only one such state, namely the (even-parity and nondegenerate) ground state, which in the nonrelativistic regime (mR not too small) likewise reduces to that found by Loudon. Operational versions of these definitions appear already in section 2.2.

Section 6 and appendices B–D investigate the one anomalous state, which develops from Loudon's nonrelativistic ground state, but eventually becomes relativistic with decreasing mR. In general E must be found numerically, and (6.3) re-writes the original eigenvalue condition (3.4)–(3.10) in terms of integrals more convenient for computing the crucial function $\beta(s)$. The main features of $\beta(s)$ are discussed in section 6.4, with plots in figures 2 and 3. Ahead of this, section 6.3 identifies the remarkable special case $s = s_1 = 1/\sqrt{1-\delta}$, which admits a simple exact solution (2.30) in closed form, with $\beta = 1$, in other words with $E/m = \sqrt{\delta} \simeq \alpha$: this suffices to show that for small enough cutoffs the binding does indeed become relativistically tight[5]. On the same tack, the fact that $E = 0$ reduces the pertinent hypergeometrics to Bessel functions allows one, in appendix B, to determine the corresponding scaled cutoff s_2 (very close to s_1) as a zero of the relatively simple combination (B.4).

[4] Though in 3D the conclusions reached by way of (i) and (ii) are generally much the same, the differences in 1D show that the physics of the two methods is not the same at all. If the physics is that of method (ii), then logically speaking it follows that not even 3D results can be justified by reasoning merely about singular potentials, no matter what matching conditions one might adopt.

[5] Dombey (2006) calls such formulae homeopathic, noting their prima facie paradoxical suggestion that no coupling at all (i.e. $\alpha \to 0$) produces very tight binding (i.e. $E/m \to 0$). The paradox stems from the fact that the limits $\alpha \to 0$ and $mR \to 0$ do not commute: homeopathism is a mirage seen when R vanishes at fixed α, but not when α vanishes at fixed R.

But the conclusion apparently least expected in the present context is that there exists another scaled cutoff s_3, only just below s_2, where E reaches a minimum value between 0 and $-m$: for $s \leqslant s_3$, the eigenvalues and thereby the eigenfunction frequencies become complex. This signals a breakdown of single-particle theory, beyond which we do not try to penetrate. Correspondingly, the curve $\beta(s)$ has a second branch, *decreasing* as s rises from s_3 to a value s_4, where E reaches the continuum threshold $-m$. The values of s and of λ at these four special points are tabulated at the end of section 6.4

The key to understanding this behaviour is that at s_3 the KG norm (2.4) changes from positive to negative, as shown in appendix C. Accordingly, for $s_3 \leqslant s \leqslant s_4$ the lower branch describes a bound *anti*particle, with charge $-e$ instead of e, but with positive energy $-E > 0$; thus the breakdown at s_3 could be initiated by the spontaneous production of bound particle plus bound antiparticle pairs, without any expenditure of energy by the agency maintaining the potential. Such scenarios are familiar in both 3D and 1D theories of KG particles experiencing strong short-range potentials, or Coulomb potentials with $\alpha \sim \mathcal{O}(1)$: references are given near the end of section 6.1. It seems strange that no earlier work has brought these studies to bear on the questions addressed in the present paper.

2. Basics

For introductions to the Coulomb KG equation in 3D we refer to the textbooks by Davydov (1965), Schiff (1968), and Bethe and Jackiw (1988), plus the early but exceptionally clear discussions by Case (1950, section 6) and Popov (1971b, section 4).

2.1. Generalities

Because $V(x)$ is even in x, we need look only at $x > 0$, and for convenience define

$$y \equiv x + R \geqslant R. \tag{2.1}$$

The wavefunction $f(y)$ obeys the same equation as does the reduced radial s-state wavefunction in 3D:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}y^2} + \left[\left(E + \frac{\alpha}{y}\right)^2 - m^2\right] f(y) = 0, \tag{2.2}$$

subject to the boundary conditions

$$f(y \to \infty) = 0, \qquad \begin{cases} f(R) = 0, & \text{(odd parity)}, \\ f'(R) = 0, & \text{(even parity)}. \end{cases} \tag{2.3}$$

Bound states are confined to

$$-m < E < m.$$

The charge density ρ and the single-particle KG norm $\mathcal{N}$ are given by

$$\mathcal{N} \equiv 2\int_0^\infty \mathrm{d}x\, \rho \equiv 2\int_0^\infty \mathrm{d}x (E - V(x)) f^2(x) = 2\int_R^\infty \mathrm{d}y \left(E + \frac{\alpha}{y}\right) f^2(y), \tag{2.4}$$

where $\mathcal{N}$ is indefinite, its sign $\varepsilon(\mathcal{N})$ indicating the charge of the particle. The frequency is $\omega = E/\hbar$; the energy is $\varepsilon(\mathcal{N})E$.

2.2. Parameters and scaling

We shall consider only

$$\alpha = 1/137 \ll 1,$$

and in forming numerical estimates take this as exact. Recall that the Bohr radius $a_B = 1/\alpha m$ is related to the reduced Compton wavelength $1/m$ and to the so-called classical electron radius r_0 by

$$1/m = \alpha a_B, \qquad r_0 = \alpha/m = \alpha^2 a_B = 2.8 \text{ fermi} = 2.8 \times 10^{-13}\text{cm}. \tag{2.5}$$

By coincidence, r_0 is comparable to nuclear radii, which in some systems might be a physically sensible choice for our cutoff R. Numerical estimates might then be based on

$$R \sim r_0 \quad \Rightarrow \quad mR \sim \alpha. \tag{2.6}$$

We define

$$\kappa = \sqrt{m^2 - E^2}, \qquad \lambda = \frac{\alpha E}{\kappa}, \qquad \frac{E}{m} = \frac{\lambda}{\sqrt{\lambda^2 + \alpha^2}}, \qquad \frac{\kappa}{m} = \frac{\alpha}{\sqrt{\lambda^2 + \alpha^2}}. \tag{2.7}$$

Thus $(\lambda = 0) \Rightarrow (E/m = 0)$ while $(\lambda \to \pm\infty) \Rightarrow (E/m \to \pm 1)$.

Further, introduce

$$z \equiv 2\kappa y, \qquad Z \equiv 2\kappa R = 2mR\frac{\alpha}{\sqrt{\lambda^2 + \alpha^2}}. \tag{2.8}$$

For instance, to study very small mR one might for simplicity choose R not as in (2.6), but so that

$$\alpha/R \gg m \quad \Rightarrow \quad \begin{Bmatrix} mR \ll \alpha, \\ Z \ll \alpha^2/\sqrt{\lambda^2 + \alpha^2} \end{Bmatrix}; \tag{2.9}$$

this could be ensured by adopting $mR \lesssim \alpha^2$, the range that will turn out to hold most surprises.

As foreseen in section 1.2, two regimes of E will prove important. *Balmer-like states* have

$$\lambda \gtrsim \mathcal{O}(1) \quad \Rightarrow \quad m - E \sim \alpha^2 m, \qquad Z \simeq 2mR\alpha/\lambda. \tag{2.10}$$

By contrast, *anomalous states* have $\lambda \lesssim \alpha$, which might include both

$$\lambda \sim \mathcal{O}(\alpha) \quad \Rightarrow \quad \{E/m \lesssim \lambda/\alpha, m - E \sim \mathcal{O}(m)\}, \qquad Z \sim \mathcal{O}(mR), \tag{2.11}$$

and

$$\lambda \lesssim \mathcal{O}(\alpha^2) \quad \Rightarrow \quad E/m \simeq \lambda/\alpha \lesssim \alpha, \qquad Z \simeq 2mR. \tag{2.12}$$

Note that (2.6) already suffices to make Z small in both cases. It remains to be determined what if any ranges of mR can realize these regimes.

With a view to the hypergeometrics that will emerge in section 2.3 we define also the parameters

$$\mu \equiv \sqrt{1/4 - \alpha^2} \equiv 1/2 - \delta, \qquad \delta = \alpha^2 + \mathcal{O}(\alpha^4) \simeq 5.328 \times 10^{-5} \ll 1. \tag{2.13}$$

Thus

$$\alpha^2 + \delta^2 = \delta, \qquad \alpha = \sqrt{\delta(1 - \delta)}, \qquad \mu - 1/2 = -\delta, \qquad \mu + 1/2 = 1 - \delta. \tag{2.14}$$

Finally, to study the ground state (which alone is anomalous) it proves convenient to scale in terms of δ rather than α, introducing

$$\beta \equiv \lambda/\delta, \qquad s \equiv mR/\delta, \qquad Z \equiv 2\delta\sigma, \tag{2.15}$$

with

$$\sigma = s\sqrt{1 - \delta}/\sqrt{1 - \delta + \delta\beta^2}. \tag{2.16}$$

2.3. Wavefunctions

The Klein–Gordon may now be re-written as Whittaker's equation

$$f''(z) + \left[-\frac{1}{4} + \frac{\lambda}{z} + \frac{(1/4 - \mu^2)}{z^2}\right] f(z) = 0. \tag{2.17}$$

The solutions are best expressed in terms of confluent hypergeometric functions M. We use the notation of Abramowitz and Stegun (1965, AS in the following) and write

$$f(z) = z^{1/2+\mu}\, \mathrm{e}^{-z/2} w(z) \tag{2.18}$$

to obtain the defining confluent hypergeometric or Kummer's equation

$$zw'' + (b - z)w' - aw = 0, \qquad \begin{aligned} a &= 1/2 + \mu - \lambda = 1 - \delta - \lambda, \\ b &= 1 + 2\mu = 2 - 2\delta, \\ 1 + a - b &= 1/2 - \mu - \lambda = \delta - \lambda. \end{aligned} \tag{2.19}$$

The solution vanishing at infinity is (AS 13.1.8 and 13.1.3)

$$w = U(a, b, z), \qquad U(a, b, z \to \infty) \sim z^{-a}, \tag{2.20}$$

$$U(a, b, z) = \frac{\pi}{\sin(\pi b)} \left\{ \frac{M(a, b, z)}{\Gamma(b)\Gamma(a - b + 1)} - z^{1-b} \frac{M(a - b + 1, 2 - b, z)}{\Gamma(a)\Gamma(2 - b)} \right\}, \tag{2.21}$$

with the derivative (AS 13.4.21)

$$U'(a, b, z) = -aU(a + 1, b + 1, z). \tag{2.22}$$

The M can be represented by power series that converge for all z:

$$M(c, d, z) \equiv 1 + \frac{c}{d} \cdot \frac{z}{1!} + \frac{c(c + 1)}{d(d + 1)} \cdot \frac{z^2}{2!} + \cdots. \tag{2.23}$$

Thus

$$f(z) = \mathrm{e}^{-z/2} z^{1/2+\mu} U(a, b, z) = W_{\lambda,\mu}(z), \tag{2.24}$$

where the W are Whittaker functions (AS 13.1.32–34). Equivalently

$$\begin{aligned} f = &-\frac{\pi}{\sin(2\pi\mu)}\, \mathrm{e}^{-z/2} \left\{ z^{1/2+\mu} \frac{M(1/2 + \mu - \lambda, 1 + 2\mu, z)}{\Gamma(1 + 2\mu)\Gamma(1/2 - \mu - \lambda)} \right. \\ &\left. - z^{1/2-\mu} \frac{M(1/2 - \mu - \lambda, 1 - 2\mu, z)}{\Gamma(1 - 2\mu)\Gamma(1/2 + \mu - \lambda)} \right\} \end{aligned} \tag{2.25}$$

$$= -\frac{\pi}{\sin(2\pi\delta)}\, \mathrm{e}^{-z/2} \left\{ z^{1-\delta} \frac{M(1 - \delta - \lambda, 2 - 2\delta, z)}{\Gamma(2 - 2\delta)\Gamma(\delta - \lambda)} - z^{\delta} \frac{M(\delta - \lambda, 2\delta, z)}{\Gamma(2\delta)\Gamma(1 - \delta - \lambda)} \right\} \tag{2.26}$$

$$= -\frac{\pi}{\sin(2\pi\delta)}\, \mathrm{e}^{-z/2} \left\{ z^{1-\delta} \frac{M(1 - \delta[1 + \beta], 2 - 2\delta, z)}{\Gamma(2 - 2\delta)\Gamma(\delta[1 - \beta])} - z^{\delta} \frac{M(\delta[1 - \beta], 2\delta, z)}{\Gamma(2\delta)\Gamma(1 - \delta[1 + \beta])} \right\}. \tag{2.27}$$

From (2.24) and (2.22) one obtains

$$\begin{aligned} f'(z) &= \mathrm{e}^{-z/2} z^{-1/2+\mu} \{[b/2 - z/2]U(a, b, z) - azU(a + 1, b + 1, z)\} \\ &= \mathrm{e}^{-z/2} z^{\delta} \{[1 - \delta - z/2]U(1 - \delta - \lambda, 2 - 2\delta, z) \\ &\quad - [1 - \delta - \lambda]zU(2 - \delta - \lambda, 3 - 2\delta, z)\}. \end{aligned} \tag{2.28}$$

It will become important that $U(a, b, z)$ and therefore f lack zeros with positive z if $a > 0$ or if $1 + a - b > 0$: see e.g. Slater (1960) and Buchholz (1969). With $\delta \ll 1$, it is the first condition that is operative, whence

$$\lambda < 1 - \delta \quad \Rightarrow \quad f(z > 0) \neq 0. \tag{2.29}$$

Finally we note the special case where $\lambda = \delta$, i.e. $\beta = 1$. Then the first terms of (2.26), (2.27) drop out and the remaining M function reduces to unity:

$$\lambda = \delta \quad \Rightarrow \quad f = \mathrm{e}^{-z/2} z^{\delta}, \qquad f' = \mathrm{e}^{-z/2} z^{-1+\delta}(\delta - z/2). \tag{2.30}$$

3. Quantization

3.1. The eigenvalue conditions

The bound-state energies are quantized by enforcing the appropriate inner boundary condition from (2.3):

$$\begin{aligned} f(Z) = 0: &\quad \text{odd parity}, \\ f'(Z) = 0: &\quad \text{even parity}, \end{aligned} \tag{3.1}$$

with $Z(\lambda, mR)$ given by (2.8).

To express these conditions in terms of the various functions M, we introduce the convenient combinations

$$\begin{aligned} A &= a = 1/2 + \mu - \lambda = -\lambda + 1 - \delta, \\ B &= a - b + 1 = 1/2 - \mu - \lambda = -\lambda + \delta; \end{aligned} \tag{3.2}$$

note that $\sin[\pi(b+1)] = -\sin[\pi b] = \sin[2\pi\delta]$; and find

$$U(a, b, Z) = \frac{\pi}{\sin(\pi b)} \left\{ \frac{M(A, 1+2\mu, Z)}{\Gamma(1+2\mu)\Gamma(B)} - Z^{-2\mu} \frac{M(B, 1-2\mu, Z)}{\Gamma(1-2\mu)\Gamma(A)} \right\},$$

$$U(a+1, b+1, Z) = \frac{-\pi}{\sin(\pi b)} \left\{ \frac{M(A+1, 2+2\mu, Z)}{\Gamma(2+2\mu)\Gamma(B)} - Z^{-1-2\mu} \frac{M(B, -2\mu, Z)}{\Gamma(-2\mu)\Gamma(A+1)} \right\}.$$

Finally we define the auxiliary function

$$j(\lambda) \equiv \frac{\Gamma(A)}{\Gamma(B)} = \frac{\Gamma(1-\lambda-\delta)}{\Gamma(-\lambda+\delta)}, \tag{3.3}$$

and can then re-cast (3.1) into relatively convenient forms. We display these along with two approximations that are adequate (i) because δ and Z are always small, and (ii) because small δ entails $1/\Gamma(2\delta) \simeq 2\delta$, as section 3.2 spells out in more detail. Then

$$j(\lambda) = \begin{cases} h(Z, \lambda): & \text{odd parity}, \\ g(Z, \lambda): & \text{even parity}, \end{cases} \tag{3.4}$$

where

$$\begin{aligned} h &\equiv Z^{-1+2\delta} \frac{\Gamma(2-2\delta)}{\Gamma(2\delta)} \cdot \frac{M_1}{M(-\lambda+1-\delta, 2-2\delta, Z)} \\ &\simeq Z^{-1+2\delta} \frac{\Gamma(2-2\delta)}{\Gamma(2\delta)} M_1 \simeq Z^{-1+2\delta} \cdot 2\delta \cdot M_1, \end{aligned} \tag{3.5}$$

$$M_1 \equiv M(-\lambda+\delta, 2\delta, Z) = M([-\beta+1]\delta, 2\delta, Z); \tag{3.6}$$

and

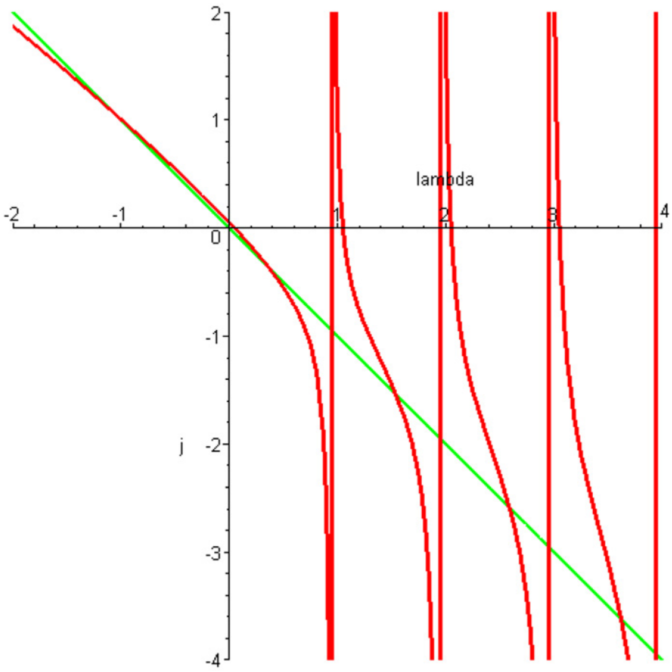

Figure 1. Horizontal axis: λ, from (2.7). Vertical axis: $j(\lambda)$, from equation (3.3), with the greatly exaggerated value $\delta = 0.05$. The straight line is $j = -\lambda$, which for realistically small values of δ and for positive λ away from the immediate neighbourhoods of poles and zeros is a close approximation to $j(\lambda)$.

$$g \equiv Z^{-1+2\delta} \frac{\Gamma(3-2\delta)}{\Gamma(2\delta)} \cdot \frac{N}{D} \simeq Z^{-1+2\delta} \frac{\Gamma(3-2\delta)}{\Gamma(2\delta)} \cdot \frac{N}{2} \simeq Z^{-1+2\delta} \cdot 2\delta \cdot N, \tag{3.7}$$

$$\begin{aligned} D \equiv \{&[1-\delta-Z/2]\,[2-2\delta]\,M(-\lambda+1-\delta, 2-2\delta, Z) \\ &+ [-\lambda+1-\delta]\,ZM(-\lambda+2-\delta, 3-2\delta, Z)\} \simeq 2, \end{aligned} \tag{3.8}$$

$$N \equiv [1-\delta-Z/2]\,M_1 - [1-2\delta]\,M_2, \tag{3.9}$$

$$M_2 \equiv M(-\lambda+\delta, -1+2\delta, Z) = M([-\beta+1]\delta, -1+2\delta, Z). \tag{3.10}$$

3.2. Poles and zeros

Regarding (3.3)–(3.7), one should keep in mind that $\Gamma(\xi)$ has no zeros, and has poles at the non-positive integers $\xi = -n = 0, -1, -2, \ldots$, with residues $(-1)^n/n!$. Thus $j(\lambda)$ has zeros at $\lambda = \delta, (1+\delta), (2+\delta), \ldots$, and poles at $\lambda = (1-\delta), (2-\delta), \ldots$; in other words it has a zero just to the right of $\lambda = 0$, and then a pole just to the left and a zero just to the right of $\lambda = 1, 2, 3, \ldots$. For positive λ well away from these points, generically so to speak, one has $j(\lambda) \simeq \Gamma(-\lambda+1)/\Gamma(-\lambda) = -\lambda$. In particular, very close to the origin

$$j\,(|\lambda| \ll 1) \simeq \delta - \lambda, \tag{3.11}$$

while near the other poles and zeros, i.e. near the positive integers,

$$\{\lambda = n - \delta + \varepsilon, n = 1, 2, 3, \ldots, \varepsilon \ll 1\} \quad \Rightarrow \quad j \simeq (2\delta/\varepsilon - 1)n \simeq (2\alpha^2/\varepsilon - 1)n. \tag{3.12}$$

Figure 1 sketches $j(\lambda)$ with the greatly exaggerated value $\delta = 0.05$, and $-\lambda$ for comparison; the verticals indicate asymptotes.

4. The structure of the spectrum: Balmer-like versus anomalous states

An overview of the spectrum is afforded by the relation (AS 13.5.8)

$$\begin{aligned} f &= \mathrm{e}^{-Z/2} Z^{1/2+\mu} \left\{ \frac{\Gamma(b-1)}{\Gamma(a)} Z^{1-b} + \mathcal{O}(1) \right\} \\ &= \mathrm{e}^{-Z/2} Z^{1/2+\mu} \left\{ \frac{\Gamma(2\mu)}{\Gamma(1/2+\mu-\lambda)} Z^{-2\mu} + \mathcal{O}(1) \right\} \\ &= \mathrm{e}^{-Z/2} \left\{ \frac{\Gamma(1-2\delta)}{\Gamma(1-\delta-\lambda)} Z^{\delta} + \mathcal{O}(Z^{1-\delta}) \right\}. \end{aligned} \tag{4.1}$$

This suffices to show that, conformably with the definitions in sections 1.2 and 2.2, the levels divide into those with $\lambda \gtrsim \mathcal{O}(1)$, which we call *Balmer-like*, and possibly others with $\lambda \ll 1$, which we call *anomalous*. It follows from (3.1) and (2.29) that all odd-parity states are Balmer-like.

Because Z is small, the first term inside the braces dominates unless the gamma function in its denominator is near a pole, i.e. unless λ is close to a positive integer $1, 2, 3, \ldots$. Elsewhere we have $f \simeq \text{const} \times \exp(-z/2) z^{\delta}$, which cannot vanish, and $f' \simeq \text{const} \times \exp(-z/2) z^{\delta} \{-1/2 + \delta/z\}$; thus f' which might vanish if z can get close to 2δ, leaving open the possibility of just one such anomalous even-parity state.

By contrast, when the gamma function *is* near a pole, these constraints cease to apply, so that Balmer-like states might exist near the points, but only near the points, where[6]

$$\lambda \simeq n + 1/2 + \mu = n + 1 - \delta, \qquad n = 0, 1, 2, \ldots, \tag{4.2}$$

$$\frac{E_n}{m} \simeq \left\{ 1 + \left(\frac{\alpha}{n+1-\delta} \right)^2 \right\}^{-1/2} = 1 - \frac{\alpha^2}{2\,(n+1)^2} + \mathcal{O}(\alpha^4). \tag{4.3}$$

We are left with two tasks. The easier task is to verify that such conventional states can actually satisfy the boundary conditions, and to determine their energies and parities. Section 5 will show that each Balmer-like level is a parity doublet, subject to weak hyperfine splitting governed by mR, with the even-parity state above the odd. (The same happens under the Schrödinger equation, as summarized in appendix A.) The harder task is to verify, in section 6, that there is also an anomalous even-parity state, and to find its energy as a function of mR. In fact the pattern of Balmer-like levels already implies that, as long as single-particle theory makes sense, there exists at least one anomalous level, because the lowest Balmer-like level is odd, whereas in our potential the ground state, if it exists, must be nodeless and therefore even.

5. Balmer-like states

5.1. Odd parity

To construct h from (3.5) one takes M_1 from (3.6); recalls that now $\lambda \sim n \gg \delta$; sets $Z \to 2mR\alpha/\lambda$, $Z^{\delta} \simeq (2mR\alpha/n)^{\alpha^2} \to 1$; and finds

$$h \simeq \frac{2\delta}{Z} - \lambda + \delta \simeq \left(\frac{\alpha}{mR} - 1 \right) \lambda. \tag{5.1}$$

[6] Close to the eigenvalues for the singular potential subject to matching conditions that ensure finite $\langle\langle V \rangle\rangle$: see appendix E.

Thus $h(\lambda)$ rises rapidly with λ, and a look at figure 1 and at (3.12) shows that it intersects $j(\lambda)$ at points where

$$\{\lambda = n - \delta + \varepsilon, n = 1, 2, 3, \ldots, \varepsilon \ll 1\} \quad \Rightarrow \quad h \simeq (\alpha/mR - 1)n = j \simeq (2\alpha^2/\varepsilon - 1)n.$$

Hence

$$\varepsilon_n(\text{odd}) \simeq 2\alpha m R, \tag{5.2}$$

independently of n, and agreeing with Loudon's nonrelativistic $\Delta\lambda(\text{odd})$ quoted in (A.3) below.

5.2. *Even parity*

Now g is given by (3.7)–(3.10), with $\lambda \simeq n \gg \delta$, and with $Z \simeq 2mR\alpha/n$. To an excellent approximation

$$g \simeq \lambda Z^{2\delta}\{-1 + \alpha^3/mR\} \simeq n\{-1 + \alpha^3/mR - 2\alpha^2 \log(n/2mR\alpha)\}. \tag{5.3}$$

Equating this to $j \simeq n\{2\alpha^2/\varepsilon - 1\}$ we obtain

$$\varepsilon_n(\text{even}) \simeq \frac{2}{\{\alpha/mR + 2\log(n/2mR\alpha)\}}. \tag{5.4}$$

In the extreme relativistic regime of *very* small mR the logarithm is negligible (i.e. in (5.3) one could then have set $Z^{2\delta} \to 1$ from the start), whence

$$\varepsilon_n(\text{even}) \simeq 2mR/\alpha \qquad (\text{relativistically}). \tag{5.5}$$

Since this exceeds $\varepsilon_n(\text{odd})$ by the large factor $1/\alpha^2$, it is indeed the even-parity state that lies higher.

By contrast, nonrelativistically the logarithm can dominate, in which case

$$\varepsilon_n(\text{even}) \simeq 1/\log(n/2mR\alpha), \qquad (\text{nonrelativistically}), \tag{5.6}$$

again in agreement with (A.3). (It is straightforward to verify that for odd parities the logarithm does not become similarly competitive.)

6. The anomalous state

6.1. *Introductory*

As discussed in section 1.1, several theoretical papers assert that the anomalous ground-state solution whether of the Schrödinger or the Klein–Gordon equation 'does not exist'; hence we proceed slowly. The problem is to determine the function $\beta(s)$ by solving $f'(Z) = 0$, in the extreme-relativistic regime[7] where $\lambda = \beta\delta \ll 1$: because δ is so small this still admits widely varying values of β. Here the writer cannot find uniformly applicable analytic approximations, and apart from three anchor points is forced to fall back on numerics. Since it proves awkward to go on looking for intersections of $j(\lambda)$ with $g(\lambda)$ (the two functions are too nearly parallel), the following subsection sets up an alternative and more manageable scheme.

Fortunately, two of the anchor points demonstrate, ahead of any elaborate numerics, that cutoffs $s \lesssim \mathcal{O}(1)$ can indeed yield anomalous ground states: namely the special case $\beta = 1$ at $s = s_1 \sim 1+$ (section 6.3), and $\beta = 0$ nearby at $s = s_2 \sim 1-$ (appendix B).

Further, we shall find that there exists a minimum cutoff s_3 (with $\beta_3 < 0$), discoverable only numerically, below which the eigenvalues become complex, and the single-particle theory

[7] For strictly practical purposes such investigations are unnecessary, because appendix A shows that even the lowest realizable cutoff stops the ground-state eigenvalue from becoming relativistic in the first place.

fails altogether (appendix C). Finally, for $s_3 \leqslant s \leqslant s_4$ (appendix D) $\beta(s)$ turns out to have another branch, with negative KG norm, indicating a bound state of an *anti*particle (coupling constant $-\alpha$ instead of α). As s approaches s_4 from below, β on this branch diverges to $-\infty$, so that the eigenvalue E_4 approaches the continuum threshold $-m$. This pattern, though it surprised the writer in the context of nominally weak 1D Coulomb potentials, is actually familiar for strong short-range KG potentials in 3D (e.g. for square wells), as discussed very clearly by Snyder and Weinberg (1940), Schiff *et al* (1940), Rafelski *et al* (1978) and Fulling (1976, 1989). For a recent illustration and for more references see Villalba and Rojas (2006). The same pattern occurs also for strong Coulomb-related 3D potentials, with $\alpha \sim \mathcal{O}(1)$, as discussed by Popov (1971a,b). What happens in 1D (unlike 3D: see Dombey 2006) is that, for any fixed α however small, the inner part of the Coulomb potential becomes effectively strong for small enough mR.

6.2. An alternative form of the eigenvalue equation

We use a representation for U valid when its first parameter and Z are positive (AS 13.2.5),

$$U(a, b, Z) = \frac{1}{\Gamma(a)} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-Zt} t^{a-1} (1+t)^{b-a-1}, \tag{6.1}$$

and the corresponding one for $U(a+1, b+1, Z)$. Substitution into (2.28) and setting $f' = 0$ then yield

$$0 = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-Zt} (1+t)^{\lambda-\delta} \{(1-\delta - Z/2) t^{-\delta-\lambda} - Z t^{1-\delta-\lambda}\}. \tag{6.2}$$

Finally we switch to $\theta = Zt$, drop some overall factors, and rearrange the result in terms of the scaled variables β and $\sigma(s, \beta)$ as

$$G_1 = G_2, \qquad \begin{pmatrix} G_1 \\ G_2 \end{pmatrix} \equiv \frac{1}{\delta} \int_0^\infty \mathrm{d}\theta\, \mathrm{e}^{-\theta} (2\delta\sigma + \theta)^{\delta(\beta-1)} \theta^{-\delta(\beta+1)} \begin{pmatrix} \{1-\theta\} \\ \{\delta(1+\sigma)\} \end{pmatrix}. \tag{6.3}$$

This is to be solved for β, given s. In the anomalous regime we assume (and can eventually verify) that s, σ, β are of order unity, or larger. It is relatively easy to see that as $\delta \to 0$ the two terms in G_1 tend to cancel: in these circumstances the factor $(1-\theta)$ of its integrand is effectively of order δ. Thus G_1 and G_2 are of comparable magnitude for small δ. The overall factor $1/\delta$ is optional; it has been introduced to facilitate numerical displays, in view of the no-cutoff limit where $\sigma = 0$ entails $(G_1, G_2) = (2, 1)\Gamma(1-2\delta) \simeq (2, 1)$.

6.3. The special case $\beta = 1$

Recall from (2.30) that $\beta = 1 \Leftrightarrow \lambda = \delta$, and that then $f(z) = \exp(-z/2) z^\delta$, while $Z = 2\delta$.

The object is to determine whether this eigenvalue can be realized, and if yes, then by what value of $s = \sigma/\sqrt{1-\delta}$. The awkward factors $(2\delta\sigma + \theta)^{\delta(\beta-1)}$ in (6.3) now reduce to unity, allowing all the integrals to be done in a closed form:

$$\begin{aligned} &\beta = 1 : G_1 = 2\Gamma(1-2\delta), \qquad G_2 = (1+\sigma)\Gamma(1-2\delta), \\ &G_1 = G_2 \quad \Rightarrow \quad \sigma = 1 \quad \Rightarrow \quad s = s_1 \equiv 1/\sqrt{1-\delta} \simeq 1 + \alpha^2/2. \end{aligned} \tag{6.4}$$

Thus we have an exact eigenvalue

$$E/m = \lambda/\sqrt{\lambda^2 + \alpha^2} = \sqrt{\delta} \simeq \alpha. \tag{6.5}$$

Appendix E.3 shows that this is the same as the lowest eigenvalue achievable in the singular potential $V = -\alpha/|x|$ if one admits divergent $\langle\langle V \rangle\rangle$, via the root q_2 of the indicial equation. Here however it is achieved in $V = -\alpha/(|x| + R)$ with finite $mR = s\delta$.

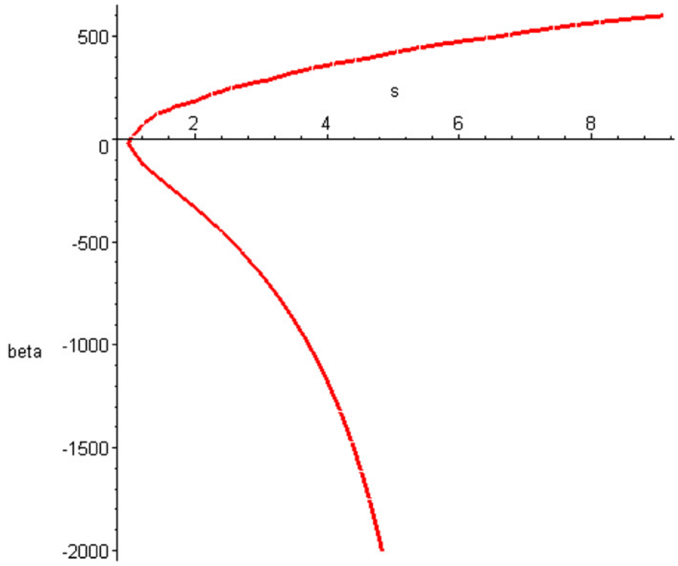

Figure 2. Horizontal axis: $s \equiv mR/\delta$. Vertical axis: $\beta \equiv \lambda/\delta$, with λ from (2.7). Low resolution plot. The vertical downward asymptote at s_4 and the last stages of the approach to it are not shown.

6.4. The function $\beta(s)$

There are two obvious ways to β: (a) select values of s, and for each find the value of β where G_1 and G_2 intersect; or (b) use the implicit-plot facility of MAPLE to plot β against s directly. The two methods cross-check satisfactorily; (a) is the more accurate, but takes longer. Figure 2 is a rough low-resolution display, with the vertical asymptote left as understood. Figure 3 is a more accurate plot of the region near and just below $s = 1$: it covers the special case just discussed, the case of zero energy, and the minimum cutoff s_3 below which the eigenvalues become complex. We comment on the main features of the curve, starting at the top right.

(i) For large enough s numerical checks confirm that the corresponding large β tally with Loudon's nonrelativistic ground states from appendix A. For instance, (6.3) with $s = 1/\alpha$ (whence $mR = \delta/\alpha \simeq \alpha$) yields $\beta = 1.416 \times 10^3$, compared to 1.428×10^3 from (A.7).

(ii) At $s_1 = 1/\sqrt{1-\delta} \simeq 1 + \alpha^2/2$ one meets the exact solution from section 6.3, with $\beta = 1$ and $E/m = \sqrt{\delta} \simeq \alpha$.

(iii) At s_2, only just below unity, the curve crosses the axis, with $\beta = \lambda = E/m = 0$. There, $f(z)$ reduces to $(z/\pi)^{-1/2} K_\mu(z/2)$, and s_2 can be located as the zero of a combination of similar functions, without further recourse to confluent hypergeometrics. The details are spelled out in appendix B.

(iv) At s_3, still very close to s_2 but now with $\beta = \beta_3 < 0$, the curve reverses, in the sense that its tangent becomes vertical ($\mathrm{d}\beta/\mathrm{d}s \to \infty$). For $s < s_3$, the eigenvalue equation (6.3) has no solutions with real λ, i.e. with real E, and thereby with real frequencies. For want of analytic approximations the value of s_3 can be determined only by trial and error, through repeated applications of method (a), with the result entered in the table below. Appendix C proves that the Klein–Gordon norm $\mathcal{N}$ changes sign at this point.

Accordingly, the lower branch of the curve, with $\lambda < \lambda_3$, has $\mathcal{N} < 0$: it describes a bound state of an antiparticle, with charge $-e$ and positive energy $-E = \Lambda/\sqrt{\Lambda^2 + \alpha^2}$, where

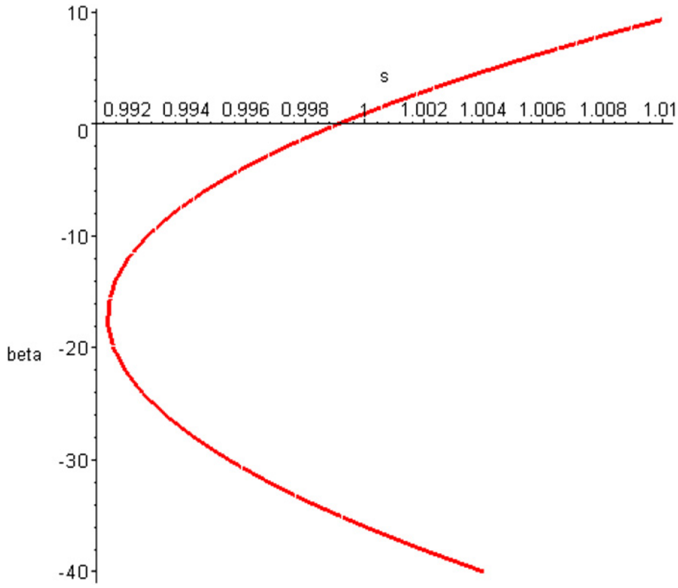

Figure 3. Horizontal axis: $s \equiv mR/\delta$. Vertical axis: $\beta \equiv \lambda/\delta$, with λ from (2.7). High resolution plot, covering the special points $\beta(s_1) = 1, \beta(s_2) = 0$, and $\beta'(s_3) \to \infty$, as discussed in section 6.4.

$\Lambda \equiv -\lambda$. At s_3 the bound particle and bound antiparticle have equal and opposite energies, and with $s \leqslant s_3$ the system is unstable against spontaneous pair creation, conformably with the normal-mode frequencies becoming complex. In other words, with small enough cutoff the system can no longer be understood on the basis of single-particle theory, and second quantization becomes unavoidable. The physics is well elucidated and referenced in the papers already cited in section 6.1.

(v) As s approaches a finite value s_4 from below, the curve approaches a vertical asymptote, i.e. $-\lambda = \Lambda \to \infty$, indicating that the energy tends to m, the threshold of the unbound antiparticle continuum. This is shown in appendix D, which also determines s_4 in terms of Bessel functions.

Tabulating these special cutoffs one has

$$\begin{aligned}
\lambda = \delta: &\quad s_1 = 1/\sqrt{1-\delta} \simeq 1.000\,027,\\
\lambda = 0: &\quad s_2 \simeq 0.999\,069,\\
\mathcal{N} = 0: &\quad 0.9913 < s_3 < 0.9914,\\
\lambda \to -\infty: &\quad s_4 \simeq 6.1712.
\end{aligned}$$

Acknowledgment

This study was prompted by discussions with Norman Dombey about his 2006 paper on the corresponding problem in 3D.

Appendix A. The nonrelativistic regime

Nonrelativistically, (2.2) is replaced by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} + Vf = E_{NR} f, \qquad E_{NR} \equiv E - m, \tag{A.1}$$

under the same boundary conditions. This problem with the potential (1.1) is solved by Loudon (1959), whose results for small R/a_B we merely quote[8], partly re-expressed in terms of our $\alpha^2 m$ instead of his e^2/a_B.

There is a Balmer-like spectrum of parity doublets ($\lambda \simeq n$ with principal quantum number $n = 1, 2, 3, \ldots$), conveniently specified by quantum defects $\delta_n \ll 1$ (not to be confused with our parameter δ) so that

$$E_{NR} = -\frac{\alpha^2 m}{2\,(n+\delta_n)^2} = -\frac{\alpha^2 m}{2n^2} + \Delta E_{NR}, \qquad \Delta E_{NR} \simeq \frac{(\alpha^2 m)\delta_n}{n^3}. \tag{A.2}$$

The splitting entails $\lambda \to \lambda + \Delta\lambda$ with

$$\begin{aligned} \Delta\lambda &= \Delta E_{NR}\frac{\partial\lambda}{\partial E} = \alpha\Delta E_{NR}\frac{m^2}{(m^2-E^2)^{3/2}} \simeq \left(\frac{\lambda}{n}\right)^3 \delta_n \simeq \delta_n, \\ \Delta\lambda(\text{even}) &\simeq \delta_n(\text{even}) \simeq \frac{1}{\log\,[n/2mR\alpha]} \gg \delta_n(\text{odd}) \simeq 2\alpha m R \simeq \Delta\lambda(\text{odd}). \end{aligned} \tag{A.3}$$

Note that in this approximation δ_n(even) depends but weakly on n, and δ_n(odd) not at all[9].

The ground-state energy is anomalous, and is governed by the transcendental equation (our ξ is Loudon's α)

$$E_{NR} = -\frac{\alpha^2 m}{2\xi^2}, \qquad (\alpha m R = R/a_B \ll 1) \quad \Rightarrow \quad \log(2\alpha m R) - \log\xi + 1/2\xi \simeq 0. \tag{A.4}$$

Thus

$$\lambda = \alpha E/\sqrt{m^2 - E^2} \simeq \alpha\sqrt{m/2E_{NR}} = \xi; \tag{A.5}$$

and, very roughly,

$$1/\xi \sim -2\log(2\alpha m R), \qquad E_{NR} \sim -2\alpha^2 m \log^2(2\alpha m R). \tag{A.6}$$

Of course, $\alpha m \to 0 \Rightarrow \xi \to 0$ and $E_{NR} \to -\infty$, which must eventually entail $|E_{NR}| \gg m$, outside the nonrelativistic domain: hence the present paper. But the divergence is only logarithmic. For instance, a quite humdrum (quasi-nuclear) $R = 1$ fermi produces only $\xi = 0.0669$ and $|E_{NR}/m| = 0.005\,96$; and very close to $R = r_0 = \alpha/m = 2.82$ fermi one finds

$$\alpha m R = \delta = 1/2 - \sqrt{1/4 - \alpha^2} \quad \Rightarrow \quad \xi = 0.0761, \qquad |E_{NR}/m| = 0.004\,60, \tag{A.7}$$

both energies being very far from relativistic.

Appendix B. Zero energy

For zero energy, the mathematics simplifies considerably. We start from

$$\lambda = 0 \quad \Rightarrow \quad Z = Z_2 = 2mR_2, \tag{B.1}$$

and exploit an exact connection between confluent hypergeometric and Bessel functions (AS 13.6.21)

$$U(1/2+\mu, 1+2\mu, Z) = \pi^{-1/2}\exp(Z/2)Z^{-\mu}K_\mu(Z/2). \tag{B.2}$$

[8] van Haeringen (1978) discusses the same equation in somewhat different and possibly more modern terms, without referring to Loudon.

[9] Loudon studies also the truncated potential $V(|x| > R) = -\alpha/|x|$, $V(|x| < R) = -\alpha/R$. When $R/a_B \ll 1$ the change makes no difference to δ_n(even) or to the ground-state energy (A.4) below, but $\delta_n(\text{odd}) \simeq 2(R/a_B)^2$ becomes second- instead of first-order small in R/a_B. There is no universal rule about which model is preferable. Though the truncated potential looks less unrealistic at large distances, there are applications where (1.1) does better by virtue of its cusp (e.g. for higher order harmonic generation by laser light: Gordon *et al* 2005).

This entails

$$f(Z) = \frac{1}{\sqrt{\pi}} Z^{1/2} K_\mu(Z/2). \tag{B.3}$$

Since all Bessel K are positive, f cannot vanish for any finite value of Z, confirming that no negative-parity state can have zero energy.

For positive-parity states one needs

$$f'(Z) = \frac{1}{2\sqrt{\pi Z}}\{(1+2\mu)K_\mu(Z/2) - ZK_{\mu+1}(Z/2)\}, \tag{B.4}$$

where we have used (AS 9.6.26) $K'_\mu(u) = -K_{\mu+1}(u) + (\mu/u)K_\mu(u)$. Solving $f'(Z_2) = f'(2s_2\delta) = 0$ numerically, one finds

$$s_2 = mR_2/\delta = 0.999\,07. \tag{B.5}$$

Appendix C. Reversal of the Klein–Gordon norm

C.1. A theorem

We study the sign $\varepsilon(\mathcal{N})$ of the Klein–Gordon norm $\mathcal{N}$ along the curve $\beta(s)$. It indicates the sign of the charge of the bound particle, while the energy of the bound state is $E\varepsilon(\mathcal{N})$. Crucially, it turns out that there exists a lowest value s_3 of s admitting a bound state, where $\mathrm{d}\beta/\mathrm{d}s \to \infty$, whence likewise $\mathrm{d}E/\mathrm{d}s \to \infty$; and at such a point $\mathcal{N}$ changes sign.

More precisely, $\mathcal{N}(s_3) = 0$ follows from a theorem about bound-state solutions

$$\{(E_\eta - V_\eta(\tau))^2 - p^2 - m^2\}\psi_\eta(\tau) = 0, \tag{C.1}$$

where η may be any parameter in V. Purely for convenience[10] we choose to fix magnitudes through

$$\int \mathrm{d}\tau\, \psi^*_\eta(\tau)\psi_\eta(\tau) = 1 \quad \Rightarrow \quad \int \mathrm{d}\tau \frac{\partial \psi^*_\eta(\tau)}{\partial\eta}\psi_\eta(\tau) + \mathrm{cc} = 0, \tag{C.2}$$

with cc standing for 'complex conjugate'; and define

$$\langle Q_\eta\rangle_\eta \equiv \int \mathrm{d}\tau\, \psi^*_\eta(\tau) Q_\eta \psi_\eta(\tau), \tag{C.3}$$

with Q_η being any operator, which may but need not depend on η. Then

$$\mathcal{N}_\eta = E_\eta - \langle V_\eta\rangle_\eta. \tag{C.4}$$

The theorem reads

$$\mathrm{d}E_\eta/\mathrm{d}\eta \to \infty \quad \Rightarrow \quad \mathcal{N}_\eta = 0. \tag{C.5}$$

It generalizes a result given by Klein and Rafelski (1975, their equation (2.17)) for the special case where η is an overall strength-factor of the potential.

[10] Looking for the sign of $\mathcal{N}$ it would obviously be perverse to try and impose $\mathcal{N} = 1$. Correspondingly, $\langle\cdots\rangle$ here is not the same as the KG expectation value $\langle\langle\cdots\rangle\rangle$ defined in appendix E.1 below.

C.2. Proof

To prove (C.5) we construct $\langle\cdots\rangle_\eta$ for (C.1), and differentiate with respect to η. Noting that $\langle E_\eta\rangle_\eta = E_\eta$ and $\langle m^2\rangle_\eta = m^2$, the result can be displayed as

$$\frac{\mathrm{d}E_\eta}{\mathrm{d}\eta}\mathcal{N}_\eta = E_\eta\frac{\mathrm{d}}{\mathrm{d}\eta}\langle V_\eta\rangle_\eta - \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\eta}\left\langle V_\eta^2\right\rangle_\eta + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\eta}\langle p^2\rangle_\eta \equiv T_\eta, \tag{C.6}$$

where

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\langle V_\eta\rangle_\eta = \left[\int \mathrm{d}\tau\,\frac{\partial\psi_\eta^*(\tau)}{\partial\eta}V_\eta\psi_\eta(\tau) + \mathrm{cc}\right] + \int \mathrm{d}\tau\,\psi_\eta^*(\tau)\left(\frac{\partial V_\eta}{\partial\eta}\right)\psi_\eta(\tau),$$

and similarly for $\mathrm{d}\left\langle V_\eta^2\right\rangle_\eta/\mathrm{d}\eta$.

In view of (C.6) it remains only to show that T_η is convergent where $\mathrm{d}E_\eta/\mathrm{d}\eta \to \infty$. We use (C.1)–(C.3) to explicate

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\langle p^2\rangle_\eta = \int \mathrm{d}\tau\,\frac{\partial\psi_\eta^*(\tau)}{\partial\eta}p^2\psi_\eta(\tau) + \mathrm{cc} = \int \mathrm{d}\tau\,\frac{\partial\psi_\eta^*(\tau)}{\partial\eta}\left(-2E_\eta V_\eta + V_\eta^2\right)\psi_\eta(\tau) + \mathrm{cc}. \tag{C.7}$$

On substitution into T_η several terms cancel, and the rest simplify to

$$T_\eta = \int \mathrm{d}\tau|\psi_\eta(\tau)|^2(E_\eta - V_\eta)\frac{\partial V_\eta}{\partial\eta}. \tag{C.8}$$

In our present problem $\eta \to R, \psi_\eta \to f, \int\mathrm{d}\tau\ldots \to \int_{-\infty}^{\infty}\mathrm{d}x\ldots$, and $V_\eta \to -\alpha/(|x|+R)$. Then T_R is convergent as long as R is finite, simply because E_R is finite, while $V_R(x) = -\alpha/(|x|+R)$ is finite for all x, and vanishes as $x \to \infty$. □

C.3. Check

To determine $\varepsilon(N)$ we can drop overall constant positive factors of $\mathcal{N}$ without comment, indicate this with arrows $\to$, and have

$$\mathcal{N} \to \int_{-\infty}^{\infty}\mathrm{d}x\,f^2(x)\{E - V\} \to \int_Z^{\infty}\mathrm{d}z\,f^2(z)\left\{\frac{\lambda m}{\sqrt{\lambda^2+\alpha^2}} + \frac{2\alpha^2 m/z}{\sqrt{\lambda^2+\alpha^2}}\right\},$$

whence

$$\begin{aligned} &\mathcal{N} \to -\mathcal{N}_1 + \mathcal{N}_2, \qquad \mathcal{N}_1 = \Lambda\int_Z^{\infty}\mathrm{d}z\,f^2(z),\\ &\mathcal{N}_2 = 2\alpha^2\int_Z^{\infty}\mathrm{d}z\,f^2(z)/z, \qquad (\Lambda \equiv -\lambda). \end{aligned} \tag{C.9}$$

Clearly $\mathcal{N}$ is positive when $\lambda \geqslant 0$, but has become negative when $\Lambda \to \infty$, i.e. when $E \to -m$. To verify that the sign changes at s_3 we choose $s = 0.991\,35$, just above s_3; from (6.3) determine the two corresponding values of $B \equiv -\beta$, call them $B_a < B_b$; and evaluate $\mathcal{N}_{a1,2}$ and $\mathcal{N}_{b1,2}$. One finds $B_a = 16.462$, $B_b = 17.925$ and

$$\begin{aligned} &\mathcal{N}_{a1} = 16.446, \qquad \mathcal{N}_{a2} = 17.174, \qquad \mathcal{N}_a = 0.728;\\ &\mathcal{N}_{b1} = 17.906, \qquad \mathcal{N}_{b2} = 17.177, \qquad \mathcal{N}_b = -0.729. \end{aligned}$$

□

Appendix D. Small Z and large $\Lambda \equiv -\lambda$

Here the eigenvalue equation $f'(Z) = 0$ is best written as

$$0 = 1 - \delta - Z/2 - (1 - \delta + \Lambda)ZU_2/U_1, \qquad Z \equiv 2mR\alpha/\sqrt{\Lambda^2 + \alpha^2}, \tag{D.1}$$

$$U_2 \equiv U(\Lambda + 2 - \delta, 3 - 2\delta, Z), \qquad U_1 \equiv U(\Lambda + 1 - \delta, 2 - 2\delta, Z). \tag{D.2}$$

We are interested in $Z \to 0$, and start by proving that this cannot happen while Λ remains convergent[11]. For if it did, then

$$U_2 \underset{Z\to 0}{\longrightarrow} -\frac{\pi}{\sin(2\pi\delta)} \cdot \frac{Z^{-2+2\delta}}{\Gamma(\Lambda + 2 - \delta)\Gamma(-1 + 2\delta)}, \tag{D.3}$$

$$U_1 \underset{Z\to 0}{\longrightarrow} \frac{\pi}{\sin(2\pi\delta)} \cdot \frac{Z^{-1+2\delta}}{\Gamma(\Lambda + 1 - \delta)\Gamma(2\delta)} \tag{D.4}$$

would reduce (D.1) to

$$0 = 1 - \delta - (1 - \delta + \Lambda)\frac{(1 - 2\delta)}{(1 - \delta + \Lambda)} = \delta: \quad \text{false.}$$

Instead, one finds that the limits $Z \to 0$ and $\Lambda \to \infty$ are linked through

$$\lim_{Z\to 0, \Lambda\to\infty} Z\Lambda = 2mR\alpha = \tilde{C}, \tag{D.5}$$

where $\tilde{C}$ is a constant: for (AS 13.3.3)

$$\lim_{c\to\infty} \Gamma(1 + c - d)U(c, d, z/c) = 2z^{1/2-d/2}K_{d-1}(2\sqrt{z})$$

and equations (D.1)–(D.4) then entail

$$0 = 1 - \delta - \tilde{C} \lim_{\Lambda\to\infty} \frac{U(\Lambda, 3 - 2\delta, \tilde{C}/\Lambda)}{U(\Lambda, 2 - 2\delta, \tilde{C}/\Lambda)} = 1 - \delta - \frac{\sqrt{\tilde{C}}K_{2-2\delta}(2\sqrt{\tilde{C}})}{K_{1-2\delta}(2\sqrt{\tilde{C}})}. \tag{D.6}$$

This determines $\tilde{C}$:

$$\tilde{C} \equiv C\delta, \qquad C = 0.090\,09 \quad \Rightarrow \quad s_4 = \frac{mR_4}{\delta} = \frac{C}{2\alpha} = 6.1712. \tag{D.7}$$

Appendix E. The singular potential

E.1. Bound-state wavefunctions and the indicial equation

With $R = 0$ from the start, (2.18)–(2.21) identify the eigenfunction that is square-integrable to $+\infty$ as

$$f(z > 0) = -\frac{\pi}{\sin(2\pi\mu)} \exp(-z/2) \left\{ z^{1/2+\mu} \frac{M(1/2 + \mu - \lambda, 1 + 2\mu, z)}{\Gamma(1 + 2\mu)\Gamma(1/2 - \mu - \lambda)} \right.$$
$$\left. - z^{1/2-\mu} \frac{M(1/2 - \mu - \lambda, 1 - 2\mu, z)}{\Gamma(1 - 2\mu)\Gamma(1/2 + \mu - \lambda)} \right\}. \tag{E.1}$$

As $z \to 0+$ the two components of f vary like $z^{1/2\pm\mu} = z^{1-\delta}$ and z^{δ}, respectively, corresponding to the two roots $q_1 = 1 - \delta$ and $q_2 = \delta$ of the indicial equation $q^2 - q + 1/4 - \mu^2 = 0$ for (2.17).

[11] Our strategy resembles Popov's (1971a, appendix A), but the tactics are different.

Since the potential is invariant under reflections, the eigenfunctions have or may without loss of generality be chosen to have definite parity ± 1, with $f(-z) = \pm f(z)$ respectively. Under (2.4) they are normalizable regardless of λ, which can therefore be determined only by imposing more restrictive criteria. Those endemic in the literature (cf the references in section 1) are much the same as for the Schrödinger equation (and/or a demand that the KG expectation value $\langle\langle V\rangle\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, \rho V \big/ \int_{-\infty}^{\infty} \mathrm{d}x \rho$ should be finite), and they are deployed with the same disregard of the implications of smoothing. Here we aim merely to register the more salient mathematical facts, without further comment on the physics beyond some final cautions voiced in section E.4.

E.2. The root q_1: finite $\langle\langle V\rangle\rangle$

Finite $\langle\langle V\rangle\rangle$ evidently requires that the second component of f be eliminated, i.e. that

$$1/2 + \mu - \lambda_n = -n, \qquad \lambda_n = n + 1/2 + \mu = n + 1 - \delta, \qquad n = 0, 1, 2, \ldots, \tag{E.2}$$

which in the nonrelativistic limit yields the Balmer spectrum (4.2).

The wavefunctions normed through (2.18) and (2.20) read

$$f_n(z > 0) = X_n\, \mathrm{e}^{-z_n/2} z_n^{1/2+\mu} M(-n, 1 + 2\mu, z_n),$$
$$X_n \equiv -\frac{\pi}{\sin(2\pi\mu)\Gamma(1 + 2\mu)\Gamma(-n - 2\mu)}, \qquad z_n = \frac{2\alpha m x}{\sqrt{\alpha^2 + \lambda_n^2}}.$$

Here M has just $(n + 1)$ terms, and (AS 13.6.9)

$$M(-n, 1 + 2\mu, z) = \frac{n!}{(1 + 2\mu)_n} L_n^{(2\mu)}(z) = \frac{1}{(1 + 2\mu)_n}\, \mathrm{e}^z z^{-2\mu} \left(\frac{\mathrm{d}}{\mathrm{d}z}\right)^n (\mathrm{e}^{-z} z^{2+2\mu}), \tag{E.3}$$

$(2\mu + 1)_n$ being Pochhammer's symbol, and $L_n^{(2\mu)}$ a generalized Laguerre polynomial (AS 22.3.9 and Erdélyi (1953)). For instance, approximating $\lambda_n \simeq n + 1$ one finds

$$f_0 \simeq \mathrm{const} \times \exp(-\alpha m x) x^{1-\delta}, \qquad f_1 \simeq \mathrm{const} \times \exp(-\alpha m x/2) x^{1-\delta} \{1 - \alpha m x/2\}. \tag{E.4}$$

Both functions vary with z on a scale of $1/\alpha m = a_{\mathrm{B}}$.

E.3. The root q_2: divergent $\langle\langle V\rangle\rangle$

By contrast, to eliminate the first and keep the second component of f on the right-hand side of (E.1) one must choose

$$1/2 - \mu - \tilde{\lambda}_n = -n, \qquad \tilde{\lambda}_n = n + 1/2 - \mu = n + \delta, \qquad n = 0, 1, 2, \ldots. \tag{E.5}$$

In the nonrelativistic limit $\tilde{\lambda}_{n+1}$ becomes degenerate with λ_n. Only $\tilde{\lambda}_0$ is anomalous:

$$\tilde{\lambda}_0 = \delta, \qquad \tilde{\beta}_0 = 1, \qquad \frac{\tilde{E}_0}{m} = \frac{\delta}{\sqrt{\alpha^2 + \delta^2}} = \sqrt{\delta} \simeq \alpha. \tag{E.6}$$

This is the solution noted by Spector and Lee (1985).

The wavefunctions normed as before read

$$\tilde{f}_n(z > 0) = \tilde{X}_n\, \mathrm{e}^{-\tilde{z}_n/2} \tilde{z}_n^{1/2-\mu} M(-n, 1 - 2\mu, \tilde{z}_n),$$
$$\tilde{X}_n \equiv -\frac{\pi}{\sin(2\pi\mu)\Gamma(1 - 2\mu)\Gamma(-n + 2\mu)}, \qquad \tilde{z}_n = \frac{2\alpha m x}{\sqrt{\alpha^2 + \tilde{\lambda}_n^2}}, \tag{E.7}$$

where $M(-n, 1 - 2\mu, \tilde{z}_n)$ can be expressed by (E.3) with $\mu \to -\mu$. For instance, approximating $\tilde{\lambda}_0 = \delta \simeq \alpha^2$ and $\tilde{\lambda}_1 \simeq 1$ one finds

$$\tilde{f}_0 \simeq \mathrm{const} \times \exp(-m x) x^{\delta}, \qquad \tilde{f}_1 \simeq \mathrm{const} \times \exp(-\alpha m x/2) x^{\delta} \{1 - m x/\alpha\}.$$

Thus $\tilde{f}_0$ varies on the scale $1/m$ of the Compton wavelength. By contrast, the exponential factor of $\tilde{f}_1$ falls only on a scale of a_B, and on this scale the second term of its polynomial factor $(1 - x/\alpha^2 a_B)$ is spectacularly enhanced relative to the first.

E.4. Caution

(i) Both the f_n and the $\tilde{f}_n$ vanish and have infinite slope as $z \to 0+$. It is sometimes inferred that because of this they can be continued to negative z only with odd parity, and that even-parity states 'do not exist'.

(ii) If for any reason one wished to keep members from both series, then one would need to face the complications of a potentially over-complete Hilbert space. For instance, we have just seen that both f_0 and $\tilde{f}_0$ are nodeless except at the origin: hence they cannot be KG-orthogonal to each other unless, arbitrarily, they are assigned opposite parities. Matching conditions chosen to make the momentum and the underlying Hamiltonian self-adjoint sidestep this problem (cf the references cited in section 1), but no such choice yet implemented fits the physics appropriate to small but finite mR.
Two discrepancies are especially fraught.

(iiia) The ground state found in section 6 is not at all akin to the eigenvalue $\tilde{\lambda}_0$, equation (E.6), allowed by the root q_2 of the indicial equation: the latter is essentially relativistic, while the former evolves continuously with decreasing mR from the nonrelativistic ground state identified in appendix A. It is mere coincidence that $\tilde{\lambda}_0$ agrees with the solution for the special cutoff considered in section 6.3: the two systems and the equations that govern them are quite different.

(iiib) Though the excited states form parity doublets, these are unconnected with the near-degeneracies between $\tilde{\lambda}_{n+1}$ and λ_n: witness the fact that both members of the doublet are close to (E.2), split by amounts independent of δ and vanishing with mR. Thus the splitting is indeed analogous to hyperfine rather than to fine structure, just as in Loudon's nonrelativistic analysis. Hence one might well have expected (correctly as it happens under a cutoff) that the odd states will turn out to be less sensitive to R than the even, simply because their wavefunctions vanish at the origin. But in this naive form the argument would apply only if the problem with $R = 0$ were well-defined, with a unique and exact solution, allowing small finite R to be treated perturbatively as an afterthought; whereas we have seen that that is not the case. On the other hand, the splittings could probably be linked to the kind of tunnelling process envisaged by Andrews, though no such calculations appear to have been attempted.

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