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Supersymmetry in second-order relativistic equations for the hydrogen atom

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Abstract. The factorisation method for constructing eigenstates and eigenvalues of the Schrödinger equation, based on the algebra of supersymmetry, is applied to second-order relativistic equations such as Kramers' equation for the Dirac-Coulomb system (hydrogen atom); the well known helicity degeneracy, for example, of the $2s_{1/2}$ and $2p_{1/2}$ levels, which is broken by the Lamb shift, is thus associated with supersymmetry. A novel form of supersymmetry is found when $l=0$: two interpenetrating ladders, founded on different and non-degenerate 'ground' states, coexist. One ladder, corresponding to a deeply bound ground state, has no counterpart in the physical hydrogen spectrum. Analogous results are obtained for the Klein-Gordon-Coulomb system in one and three dimensions. Eigenstates and eigenvalues for the one-dimensional Dirac-Coulomb system are found by projection.

1. Introduction

Supersymmetry affords an elegant interpretation of the level degeneracies of a Dirac electron both in a constant magnetic field (Khare and Maharana 1984, Blockley and Stedman 1985) and also in the hydrogen atom, or 3D Dirac-Coulomb system (Sukumar 1985a). It is curious that the accurate prediction of the breakdown of each of these degeneracies, by the anomalous g factor and the Lamb shift respectively, are historically major triumphs of QED. This supersymmetry of a Dirac electron in the field of an electric monopole parallels a supersymmetry in the field of a magnetic monopole (d'Hoker and Vinet 1984, 1985a, b, c, Yamagishi 1984). A unified relativistic formulation would be of interest; see also Ui (1984), Balantekin (1985) and Niemi (1985).

In the 3D Dirac-Coulomb system, described by $O_-\psi=0$ (§ 2), Sukumar's (1985a) construction centres on the coupled first-order radial equations. We give a different approach based on Kramers' equation ($O_-O_+\psi=0$; see Biedenharn and Horwitz 1984). The associated second-order radial equation may be cast in scalar form (§ 2), and is then particularly amenable to the standard application of supersymmetric quantum mechanics (Gendenshtein 1983, Andrianov *et al* 1984a, b, c, 1985, Sukumar 1985b, c, Stedman 1986). Indeed its supersymmetric solution has close affinities with the non-relativistic Coulomb system as well as the Klein-Gordon-Coulomb system (§ 4). However the details of the construction (§ 3) require a careful discussion of alternative parametrisations of the supersymmetry generator, and also reveal a new feature: for zero orbital quantum number l, there are two interpenetrating supersymmetric ladders of solutions, based on different and non-degenerate 'ground' states. One of these states

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is essentially the 1s ground state of the physical hydrogen atom. The other is deeply bound ($E_0^* \sim \alpha m_0 c^2$) and strongly peaked at the origin ($\psi_0^* \sim \exp(-r/\lambda_c)$, where λ_c is the Compton wavelength). The ladder of eigenstates built upon this state, while valid solutions of Kramers' equation, have no physical counterpart in the hydrogen atom; the corresponding eigenstates of the first-order equation (the projections $O_+\psi_n^*$, $n = 0, 1, \ldots$) are non-normalisable (§ 5). Corresponding results hold (§ 4) for the (3D) Klein-Gordon equation with either a 1D ($1/|x|$) or 3D ($1/r$) Coulomb potential; we refer to these for brevity as the 1D and 3D Klein-Gordon-Coulomb systems respectively. Similarly the projected eigenstates appropriate to the 1D Dirac-Coulomb system may be constructed, and those corresponding to the deeply bound state are non-normalisable (§ 5).

The physical interest of these deeply bound states, and so the associated ladders of solutions, has been controversial. Loudon (1959) found such a state in the 1D non-relativistic Coulomb system (the Schrödinger equation with a $1/|x|$ potential); for the debate on its significance, see the references of Spector and Lee (1985). Loudon also found a double degeneracy of all excited levels, the degenerate states having opposite parity. Imbo and Sukhatme (1985) pointed out that this degeneracy has a simple interpretation in supersymmetric quantum mechanics: the partner supersymmetric Hamiltonians are identical. Indeed the above-mentioned ladders are analogous to the odd- and even-parity solutions of Loudon (1959) (§ 4). Again the physical applicability has been debated (McIntosh 1971, Spector and Lee 1985). Certainly one-dimensional equations with Coulomb potentials have a practical application. One-dimensional Coulomb systems have been realised experimentally in 1D fabricated semiconductor devices (see Spector and Lee 1985), and also for charges interacting with their images in the surface of liquid helium (Grimes *et al* 1976, Poitrenaud and Williams 1972, 1974). The observed spectrum corresponds to excited state transitions, and surface effects are certain to modify any physical interpretation of the deeply bound states. Our (apparently novel) solution of the 1D Dirac-Coulomb system confirms the absence of the deeply bound state for a spin-$\frac{1}{2}$ particle in a 1D Coulomb potential. We also consider the 3D Klein-Gordon-Coulomb system, which describes pionic and kaonic atoms. The Klein-Gordon fine structure has been observed (see the references in Friar and Tomusiak 1984), although only in highly excited states; strong interaction effects will certainly modify (probably unrecognisably) the most optimistic attempts to give a physical significance to the deeply bound state in this system.

We now briefly review the standard application of supersymmetric quantum mechanics. For every non-relativistic system whose Schrödinger equation contains a potential $V(r)$, we may create another with a Schrödinger equation whose potential $V'(r)$ may differ, but whose eigenvalues are in (nearly) 1:1 correspondence. We write the original Schrödinger equation $H\psi = [-(\hbar^2/2m)\nabla^2 + V]\psi = E\psi$ in the form

$$H\psi = (A^+A + \varepsilon)\psi = E\psi, \tag{1}$$

by the construction

$$A \equiv [\hbar/(2m)^{1/2}][-\nabla + (\nabla \ln \psi_0)], \qquad \varepsilon \equiv E_0 \tag{2}$$

E_0, ψ_0 being the ground-state energy and wavefunction. The supersymmetric counterpart is then $H'(A\psi) \equiv (AA^+ + \varepsilon)(A\psi) = E(A\psi)$. As the above construction shows, H and H' have common eigenvalues. (If H and H' are each of physical interest, the

degeneracy also has physical interest.) Supersymmetry gives a fundamental interpretation of this degeneracy. The supersymmetry generator Q

$$Q \equiv \begin{bmatrix} 0 & 0 \\ A & 0 \end{bmatrix},$$

is nilpotent and corresponds to a Hamiltonian $\boldsymbol{H} \equiv \{Q, Q^+\}$ which is supersymmetric ($[\boldsymbol{H}, Q] = 0$) and which contains $H' - \varepsilon$ and $H - \varepsilon$ in block diagonal form. The 'bosonic' (say H) sector and 'fermionic' (H') sector have paired degenerate eigenstates coupled by Q (i.e. by A), except for the zero-energy ground state (of $H - \varepsilon$), which is non-degenerate (e.g. Blockley and Stedman 1985).

An application of these ideas to the radial equation for the non-relativistic hydrogen atom generates radial operators for adjacent l values (but the same potential) as supersymmetric partners. Hence this supersymmetry implies the l independence of the eigenvalues traditionally associated with the O(4) symmetry of this problem (Sukumar 1985a). (The application detailed by Kostelecky and Nieto (1984) is identical to this in principle. However it is unhelpful to say, for example, that supersymmetry links s states to s states, p to p, etc; in the first analysis, this supersymmetry algebra links systems of levels for which $\Delta l = 1$. Their application is extended and related work is reviewed in Kostelecky *et al* (1985).)

The factorisation technique has been applied in the case of the relativistic hydrogen atom to the second-order radial equation by Green (1965), and (including the link with supersymmetry) to the coupled first-order radial equations by Sukumar (1985a). It is the first method in particular which has close affinities with the above discussion, and which we shall emphasise in this paper. The second-order radial equation for the (relativistic) Dirac hydrogen atom may be cast into a Schrödinger-like form; the only change is the redefinition of a few scalar parameters, provided (see § 2) we work in the eigenbasis of the operator Λ where

$$\begin{aligned} \Lambda &\equiv K/\hbar + \mathrm{i}\alpha\boldsymbol{\alpha} \cdot \hat{\boldsymbol{r}} \\ K &\equiv -(\boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar). \end{aligned} \tag{3}$$

In these equations $\{\boldsymbol{\sigma}\}$ are the Pauli matrices, $\{\gamma_\mu\}$ the Dirac matrices, $\alpha \equiv e^2/2hc\varepsilon_0$ is the fine structure constant, the caret denotes a unit vector and $\boldsymbol{\alpha} = \gamma_0\boldsymbol{\gamma}$ ($\gamma_0 = \beta$). Λ is called the Temple operator (and is written as Γ) by Biedenharn (1983), and is called the Martin-Glauber (L) or Johnson (J) operator by other authors. We note in passing (see § 2) that the eigenvalues κ of the operator K (equation (3)) have equal magnitude and opposite sign ($\kappa = \pm|\kappa|$) in the two states of each excited level for given j, i.e. in the states $n(l-1)_j$, nl_j, where $l = |\kappa|$, $j = |\kappa| - \frac{1}{2}$, and that these states are degenerate (the helicity degeneracy) since the energy is independent of $\mathrm{sgn}(\kappa)$ (figure 1). For any choice of j, the energy level structure of the Dirac atom, apart from an overall shift in energy, has precisely the standard form of a supersymmetric spectrum—a non-degenerate ground state, and doubly degenerate excited states. In addition, factorisation of the second-order radial equation (Green 1965) introduces operators analogous to A which ladder between radial wavefunctions with opposite signs of κ, and from which the radial eigenfunctions may be obtained in principle by an *aufbau* technique (Green 1965), as in the general method referenced above. (This ladder operator is related to the operators variously called the Coulomb helicity operator or the Lippmann-Johnson operator—cf equation (69) of Biedenharn (1983) for example—as we confirm in § 5.) All this indicates strongly that this degeneracy may be attributed

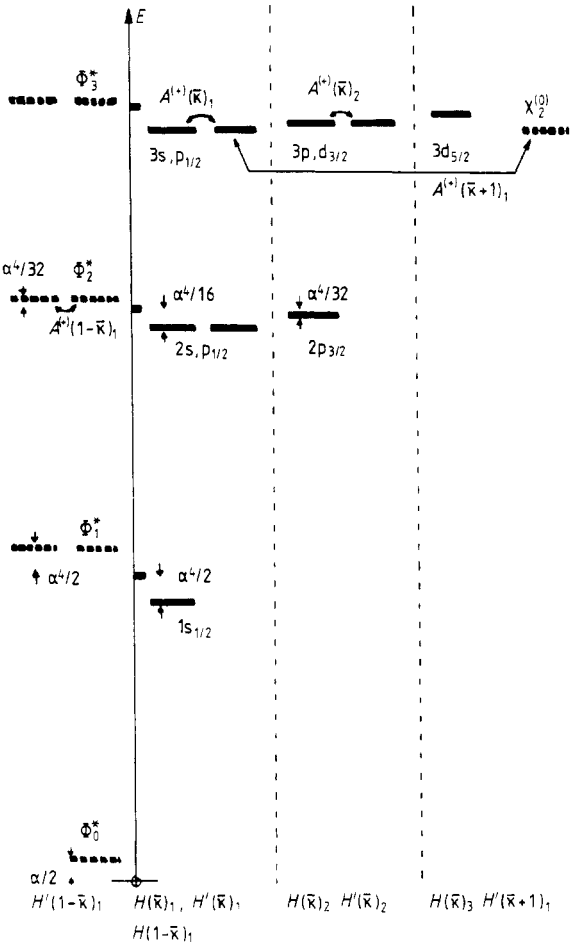

Figure 1. Schematic energy level scheme (not to scale) for the 15 lowest energy solutions of Kramers' equation; these form initial states of various supersymmetric hierarchies as discussed in the text. Full lines denote solutions corresponding to physical positive-mass solutions of the first-order Dirac equation. Negative-mass counterparts (see figure 1 of Martin and Glauber (1958)) are not depicted. Markers on the vertical axis represent level positions ($N = 1, 2, 3$) in the absence of fine structure; some fine structure splittings are indicated in units of m_0c^2. The action of various ladder operators are illustrated, and relevant Hamiltonians $H(p)$, $H'(p)$ are given at the foot of each column; in each case subscripts denote the relevant value of $|\kappa|$.

to supersymmetry in essentially the same manner as for the non-relativistic hydrogen atom. It appears as if this supersymmetry should result from a trivial application of the general formulation to the second-order radial equation for the relativistic hydrogen atom.

However, some differences of principle between the solutions of the relativistic and non-relativistic second-order equation complicate the demonstration. First, we no longer have O(4) symmetry, the analogue of l in the radial equation is not an integer and the parameters in the radial equation are level-dependent. Second, the operator Λ is non-Hermitian; in addition, it does not commute with the Dirac Hamiltonian. The interpretation and the factorisation procedure are greatly complicated by the Λ-diagonalising transformation, which parallels a transformation in the Sommerfeld

theory rather than anything in the non-relativistic quantum theory (Biedenharn 1962, 1983). Third, novel factorisations may be found even for familiar equations, by judicious choice of parameters. For example, in their analysis of the types of potential which will give the observed level ordering in charmonium, Grosse and Martin (1984) discuss new factorisations of the harmonic oscillator radial equation. (Their D factorisation is a puzzling claim; it fails to satisfy the stated properties, and indeed there seems to be no *a priori* motive for introducing it since the symmetry they find in their equation (27) could equally well be achieved from the Hermitian conjugate of their equation (25).) Fourth, only (admixed versions of) the eigenfunctions Φ of the (second-order) Kramers' equation are eigenfunctions Ψ of the (first-order) Dirac equation, and to judge from figure 1 of Martin and Glauber (1958) only some of the related degeneracies are of physical interest. In retrospect, we find a further difference: the existence of the deeply bound solution (together with the associated ladder of eigenstates) of the Kramers', but not the Dirac, equation.

2. Kramers' equation

The 3D Dirac-Coulomb equation for the hydrogen atom has the form $O_-\Psi = (\not{p} - m_0 c)\Psi = 0$, where $\not{p} \equiv \gamma_\mu (p^\mu - qA^\mu)$, $p_\mu \equiv i\hbar\,\partial_\mu$, $qA^0 = -\alpha\hbar c/r$ (for other atoms than hydrogen, $\alpha \to Z\alpha$). Ψ, being a positive mass solution, has zero negative mass projection; the positive and negative mass projection operators are

$$O_\pm \equiv c(\not{p} \pm m_0 c^2) = c\boldsymbol{\gamma}\cdot\boldsymbol{p} + \gamma_0(E + \alpha\hbar c/r) \pm m_0 c^2$$

where we use a metric $(+---)$ and where $E \equiv i\hbar\,\partial_t$. We shall solve Kramers' equation:

$$O_- O_+ \Phi = 0 = O_+ O_- \Phi. \tag{4}$$

Eigenstates Ψ for the 3D Dirac-Coulomb system are derived by projection: $\Psi \equiv O_+\Phi$ (§ 5).

With the substitution $\boldsymbol{p}^2 = (1/r)p_r^2 r + \boldsymbol{L}^2/r^2$ (where $p_r = \hat{\boldsymbol{r}}\cdot\boldsymbol{p} = -i\hbar\,\partial_r$) Kramers' equation reduces to the form

$$[\partial^2/\partial r^2 - (K^2 - \alpha^2 + \Lambda)/r^2 + 2\alpha E/\hbar c r - k^2](r\Phi) = 0 \tag{5}$$

where $k \equiv (m_0^2 c^4 - E^2)^{1/2}/\hbar c$.

The operators $\boldsymbol{J} \equiv \boldsymbol{L} + (\hbar/2)\boldsymbol{\sigma}$, βK, and $O_\pm$ mutually commute; Λ commutes with βK, K^2, $\boldsymbol{J}$ and $O_- O_+$ but not with K or $O_\pm$. Nevertheless the eigenbasis of Λ (the 'Biedenharn' basis) is particularly convenient, since the operator in equation (5) becomes a scalar. (This basis has also proved convenient for the solution of the Dirac-Coulomb problem by path-integral methods (Kayed and Inomata 1984).) Note that although Λ is non-Hermitian, its eigenvalues are real (Martin and Glauber 1958) and the required transformation of basis is unitary (Biedenharn 1983); we shall use right eigenvalues and eigenstates of Λ throughout. The eigenstates Φ of Kramers' equation can be labelled by their energy and by the eigenvalues $j(j+1)\hbar^2$, $m_j\hbar$, $\hbar\kappa$, λ of the operators $\boldsymbol{J}^2$, J_z, βK, Λ, respectively. The eigenstates of the Dirac equation, $\Psi = O_+\Phi$, are labelled by the eigenvalues of $\boldsymbol{J}^2$, J_z and βK, but the projection O_+ will admix eigenstates of Λ (§ 5).

K anticommutes with $\boldsymbol{\alpha}\cdot\hat{\boldsymbol{r}}$ (and with $\boldsymbol{\alpha}\cdot\boldsymbol{p}$). This has three consequences of immediate interest. First, as mentioned above, K and Λ do not commute. Second, K^2 and Λ do commute and the operator in equation (5) is a scalar in the Biedenharn basis. Third, $\Lambda^2 = K^2/\hbar^2 - \alpha^2$; this gives the useful form $\Lambda(\Lambda+1)$ to the numerator of

the centrifugal term in equation (5), and also gives the relation $\lambda = \pm\bar{\kappa}$ where $\bar{\kappa} \equiv +(\kappa^2 - \alpha^2)^{1/2}$, between the eigenvalues λ and $\hbar^2\kappa^2$ of Λ, K^2. The connection between $\mathrm{sgn}(\kappa)$ and $\mathrm{sgn}(\lambda)$ (sgn is the sign function) will be discussed in § 5.

The angular part of the solution, in particular the algebra of the angular momenta $\boldsymbol{J}$, $\boldsymbol{L}$ (Margeneau and Murphy 1968, Messiah 1962) gives $j = \frac{1}{2}, \frac{3}{2}, \ldots, l = 1, 2, \ldots$ ($\boldsymbol{L}^2 = l(l+1)\hbar^2$). Since $\boldsymbol{J}^2 = K^2 - \hbar^2/4$, $j = |\kappa| - \frac{1}{2}$; any one of j, $|\kappa|$ or $\bar{\kappa}$ determines the other two. Hence $\kappa = \pm 1, \pm 2, \ldots$. Also, since $\boldsymbol{L}^2 = K^2 + \hbar K = \beta K(\beta K + \hbar\beta)$, $l(l+1) = \lambda(\lambda \pm 1)$, $+(-)$ for upper (lower) components ($\langle\beta\rangle = 1(-1)$). For the upper components, then, we may identify $l = |\kappa| + \frac{1}{2}(\mathrm{sgn}(\kappa) - 1)$ as the conventional orbital quantum number for the Dirac solution.

3. Supersymmetric construction of solutions of Kramers' equation

We write the scalar form of equation (5), changing the normalisation for convenience, as

$$[-\mathrm{D}^2 + \lambda(\lambda+1)/y^2 - 1/y]\Omega = -(1/4\eta^2)\Omega \tag{6}$$

where $\mathrm{D} \equiv \partial/\partial y$, $y \equiv 2\eta kr$, $\eta \equiv \alpha E/\hbar ck$ and $\Omega(y) \equiv y\Phi(r)$. We now solve for both eigenstates and eigenvalues of equation (6) using the supersymmetry approach to the Schrödinger equation. As Green (1965), for example, comments, equation (6) has the same form as the non-relativistic analogue. It does not follow that its solutions also have the same form; λ is irrational and non-positive, and this affects the construction of normalised wavefunctions.

We seek a factorisation of equation (6) as in equation (1), and try the form

$$\begin{aligned} A(p) &\equiv -\mathrm{D} + p/y - q \\ H(p) &= A^{+}(p)A(p) + \varepsilon(p) \\ &= -\mathrm{D}^2 + p(p-1)/y^2 - 2pq/y + \varepsilon + q^2. \end{aligned} \tag{7}$$

This requires $p(p-1) = \lambda(\lambda+1)$, $q = q(p) = 1/2p$, $\varepsilon = \varepsilon(p) = -q^2$. The first condition gives two roots: $p^{(1)} = -\lambda$, $p^{(2)} = \lambda + 1$. The other conditions give $\eta = p$ for the ground state since the analogue of the ground-state energy ε of § 1 is the eigenvalue $-1/4\eta^2$ of equation (6) and since η is positive by definition (as explained below, p is positive).

The ground state Ω_0 for any choice of λ is given (cf equations (1) and (2)) by the constraint $A\Omega_0 = 0$. This constraint gives $\Omega_0 \propto y^p \exp(-qy)$. For normalisability at infinity, q must be positive. For normalisability at the origin, we require in three dimensions convergence of the integral $\int (\Omega_0(y)/y)^2 \, \mathrm{d}\tau$, and in one dimension convergence of the integral $\int \Omega_0(y)^2 \, \mathrm{d}y$, i.e. in each case $p > -\frac{1}{2}$. Together, these conditions require that p be positive, since $q = 1/2p$. (In § 5 we shall see that not all normalisable solutions of Kramers' and related equations are also normalisable on projection for the Dirac equation, since the projector O_+ introduces a factor y^{-1}.)

The root $p^{(1)}$ is positive as required only for negative λ ($\lambda = -\bar{\kappa}$). With a particular choice of $|\kappa|$, and with this choice of Hamiltonian ($p = \bar{\kappa}$) we obtain one sector (say bosonic) of a supersymmetric hierarchy as the eigenstates of $H(\bar{\kappa})$. The ground state becomes $\Omega_{0,|\kappa|,-} \propto y^{\bar{\kappa}} \exp(-y/2\bar{\kappa})$. (We label eigenfunctions by $\Omega_{n,|\kappa|,\mathrm{sgn}(\lambda)}(y)$ where the integer n labelling the eigenstates for states of given λ (i.e. of given $|\kappa|$, $\mathrm{sgn}(\lambda)$) increases with energy from zero.) $H(\bar{\kappa})$ then describes all states of given $\bar{\kappa}$ with $\lambda < 0$; all these are appropriate for the numerator $\bar{\kappa}(\bar{\kappa} - 1)$ of the $\mathrm{O}(y^{-2})$ term in $H(\bar{\kappa})$. In

contrast, the root $p^{(1)}$ was of no interest in the non-relativistic solution since l, the analogue of λ, is non-negative (see however § 4).

The supersymmetric partner $H'(p) = AA^+ + \varepsilon$ is uniquely defined given a choice of p as above, and the $O(y^{-2})$ term has the numerator $p(p+1)$. If we wish to identify $H'(p)$ as a Hamiltonian of physical interest in the context of our problem, we must identify the numerator $p(p+1)$ with the (physically interesting) form $\lambda(\lambda+1)$ in equation (6), perhaps with a different value of λ, say μ: $p(p+1) = \mu(\mu+1)$. This assignment in turn has multiple solutions: $\mu^{(1)} = p$, $\mu^{(2)} = -(p+1)$. For $p = p^{(1)}$, $\mu^{(2)} = -(\bar{\kappa}+1)$ and has no direct physical interest since it cannot correspond to some $\pm\bar{\kappa}'$. However the choice $\mu^{(1)} = \bar{\kappa}$ gives $H'(\bar{\kappa})$ the relevance of describing all states with this $\bar{\kappa}$ and with $\lambda > 0$. We label these in the same way as before, with n commencing at zero for the state of lowest energy. This establishes the other (fermionic) sector of the supersymmetric hierarchy as the set of states with the same $\bar{\kappa}$, but opposite λ. Hence by supersymmetry the states $\Psi_{n,|\kappa|,-}(y)$, $\Psi_{(n-1),|\kappa|,+}(y)$ with given η, $\bar{\kappa}$ but opposite values of $\mathrm{sgn}(\lambda)$ are degenerate in the Dirac hydrogen atom (figure 1). This gives helicity-conjugate states (for example, the levels split by the Lamb shift) their familiar degeneracy; the projected states with opposite values of $\mathrm{sgn}(\kappa)$ are admixtures of the above states and so also degenerate (§ 5).

We now discuss the root $p^{(2)}$. $p^{(2)}$ is also positive if $\lambda > -1$. This includes all the values $\lambda > 0$, when $p^{(2)} = \bar{\kappa}+1$ and $H(p^{(2)})$ has the same (previously fermionic, now bosonic) solutions as discussed above for $H'(\bar{\kappa})$. This gives no new result; $H'(\bar{\kappa}+1)$ contains the physically uninteresting numerator $(\bar{\kappa}+1)(\bar{\kappa}+2)$ so that the new fermionic solutions do not correspond to the Dirac–Coulomb problem. By way of contrast, it was just this root which was of interest in the non-relativistic problem; here, however, $\bar{\kappa}$ is irrational. Nevertheless, we shall find a constructional value in these unphysical Hamiltonians.

The root $p^{(2)}$ also includes the curious special case $p = p^* \equiv 1-(1+\alpha^2)^{1/2}$, corresponding to an eigenstate Ω_0^* with $\lambda < 0$, $\kappa = -1$, with the same quantum numbers as the $1s_{1/2}$ state ($|\kappa| = 1$, $\mathrm{sgn}(\lambda) = -1$), but with a greatly different wavefunction: $\Omega_0^* \propto y^{p^*}\exp(-y/2p^*) \approx y^{\beta/2}\exp(-y/\beta)$ ($\beta \equiv \alpha^2$; note that $y/2p^* \approx r/\lambda_c$) and energy (cf equation (8)) $E^* = m_0c^2(p^*/2)^{1/2} = \frac{1}{2}m_0c^2[(1+\alpha)^{1/2}-(1-\alpha)^{1/2}] \approx \alpha m_0c^2/2$, corresponding to the choice $\varepsilon_0^* = -1/4p^{*2}$. This positive energy and normalisable solution of Kramers' equation (figure 1) seems not to have been noted before, though it is equally accessible from the series solution and similar states have been discussed in other systems (§ 4). Fortunately for the hydrogen ground state (or perhaps unfortunately for the SDI initiative), there is no corresponding solution for the first-order Dirac equation (see § 5); there, the series solution requires $p = \bar{\kappa}$ for positivity in the ground state.

This solution clearly differentiates the application of the factorisation procedure to the first-order radial equations (Sukumar 1985a) and to Kramers' equation, and serves as a graphic illustration of the qualitative difference between the relativistic and non-relativistic applications of equation (6).

Ω_0^* is the lowest energy state of an infinite set of solutions forming one sector of a supersymmetric ladder, interleaving the states in the ladder based on $\Omega_{0,1,-}$. Kramers' equation has this peculiar feature, not anticipated in previous discussions of supersymmetry in quantum mechanics, of admitting two non-degenerate nodeless functions of the form $y^p\exp(-qy)$, each of which may form the basis of a simple factorisation scheme. We shall compare these two hierarchies shortly, but note here that since $\varepsilon_0^* = \varepsilon(1-\bar{\kappa}) \ll \varepsilon(\bar{\kappa})$, although Ω_0^* is an eigenstate of the *positive* definite operator

$A^+(\bar\kappa)A(\bar\kappa)$, its eigenvalue is *negative*. The essential feature which was lacking in earlier discussions is that only one of the states formed by the action of the ladder operators A, A^+, need be normalisable. In our case neither $A(\bar\kappa)\Omega_0^*$ nor $A(1-\bar\kappa)\Omega_{n,1,-}$ are normalisable, and so not all excited eigenstates have degenerate partners.

We now iterate this construction following Gendenshtein (1983) and Sukumar (1985a, b, c), to generate all the bound-state wavefunctions. (For given $\bar\kappa$ (or j, or $|\kappa|$) these are contained in $H(\bar\kappa)$ and $H'(\bar\kappa)$, for $\lambda<0$ and $\lambda>0$ respectively.) We generate an infinite chain $\{H_m|m=0,1,\ldots\}$ of Hamiltonians, each lacking the ground state of its predecessor, with adjacent Hamiltonians defined by equation (7) where $H\to H_m$, $H'\to H_{m+1}$, $A\to A_m$, $\varepsilon\to\varepsilon_m$, our previous analysis applying to $m=0$. For $m>0$ we must choose the only positive root $p=p_m\equiv\bar\kappa+m$; $A_m\equiv A(p_m)$ and $\varepsilon_m=\varepsilon(p_m)$. This results in formally the same Hamiltonian hierarchy as in the non-relativistic case. The necessity of considering non-physical Hamiltonians for $m>1$ is no impediment to the method, which is now purely one of construction. The lowest eigenvalue ε_m of H_m equals the eigenvalue $-1/4\eta^2$ of equation (6) if $\eta=\eta_m=\bar\kappa+m$; hence (from the earlier definitions of η and k) we have the energy eigenvalues

$$E_m=m_0c^2/[1+(\alpha/\eta_m)^2]^{1/2} \tag{8}$$

of the Hamiltonian H (and H') directly (Green 1965). The principal quantum number N is therefore $|\kappa|+m$, the nearest integer to η_m.

We obtain similarly an analytic derivation of the eigenfunctions. With this choice of η_m, the ground state $\chi_m^{(0)}$ of H_m is given from equations (2) and (7) as $\chi_m^{(0)}\propto y^{p_m}\exp(-y/2p_m)$. The excited states $H_0=H(\bar\kappa)$ (or $H_1=H'(\bar\kappa)$) are given by applying n operators A_i^+ on this state, converting between supersymmetric partners in each pair of adjacent Hamiltonians:

$$\begin{aligned}\Omega_{n,|\kappa|,+}&\propto A_1^+A_2^+\ldots A_n^+\chi_n^{(0)}\\ \Omega_{n+1,|\kappa|,-}&\propto A_0^+\Omega_{n,|\kappa|,+}.\end{aligned} \tag{9}$$

This construction is paralleled in the factorisation approach of Green (1965), but is more complete since the ground states $\chi_m^{(0)}$ are also determined by the supersymmetry argument (more exactly, by equation (2)), solving the eigenfunction problem for all bound states completely and elegantly (Sukumar 1985a).

Since each application of A_i^+ creates a node in the radial wavefunction (Baumgartner *et al* 1984), n is also the number of nodes; from equation (9), $m=n+\frac{1}{2}(1+\mathrm{sgn}(\lambda))$. With $\eta_m=\bar\kappa+m$, $N=|\kappa|+m$ this defines all bound-state quantum numbers, energies (equation (8)) and eigenfunctions (equation (9)).

A similar form for the eigenfunctions is given by Martin and Glauber (1958) ($x\equiv 2kr$, $a\equiv\bar\kappa+m-n$):

$$\begin{aligned}\Omega_{n,|\kappa|,\mathrm{sgn}(\lambda)}(x)&\propto x^{1-a}\,\mathrm{e}^{x/2}(\partial/\partial x)^n(x^{n+2a-1}\,\mathrm{e}^{-x})\\ &=[\partial/\partial x+(a-1)/x-\tfrac{1}{2}]^n(x^{n+a}\,\mathrm{e}^{-x/2}).\end{aligned}$$

This may be verified from equation (9) by contour integration (C V Sukumar, private communication).

A similar derivation may be made for the additional solutions Ω_n^* associated with $p^*=1-\bar\kappa$, when $\lambda=-\bar\kappa$, $|\kappa|=1$ (the asterisk in this context distinguishes parameters relevant to this case, and does not mean complex conjugation). The Hamiltonian $H_0^*=H(1-\bar\kappa)$ has as its supersymmetric partner $H_1^*=H'(1-\bar\kappa)=H(2-\bar\kappa)$. Iterating

as before, $p_m^* = p^* + m$, and we have the further excited states for Kramers' equation

$$\Omega_n^* \equiv A_0^{*+} A_1^{*+} \ldots A_n^{*+} \tilde{\chi}_n^{(0)} \tag{10}$$

where in all definitions $p_m \to p_m^*$; similarly, in equation (8).

4. Supersymmetric solutions of other second-order relativistic equations in Coulomb systems

4.1. Introduction: non-relativistic limit

Several equations may be cast in the form (generalising equation (6))

$$(-\mathrm{D}^2 + N/y^2 - \zeta/y)\Omega = -(1/4\eta^2)\Omega \tag{11}$$

where $\mathrm{D} \equiv \partial/\partial y$, $\zeta \equiv \mathrm{sgn}(y)$ (in 1D problems). The supersymmetric analysis has the standard form of equation (7), with $q \to \zeta q$, $p(p-1) = N$, and with $\eta_m \equiv p_m \equiv p + m$ defining the standard hierarchy of Hamiltonians and eigenvalues.

For example, in the non-relativistic case, the 3D Coulomb system has the above form with $N = l(l+1)$, $\Omega \equiv y\Phi$, $y \equiv 2\alpha r/\lambda_c$, $\eta^2 \equiv -\alpha^2 m_0 c^2/2E$, and the 1D Coulomb system has an analogous form with $N = 0$, $\Omega \equiv \Phi$, $y \equiv 2\alpha x/\lambda_c$, which is formally the same equation with $l = 0$. If the 1D equation has an infinitely bound ground state, then so does the 3D equation; these possibilities correspond to the alternative parametrisation of § 3 in which $p = p^{(2)} = -l$; for $l = 0$ this has the marginal value of zero, and one might define $A(p) \equiv -\mathrm{D} + p/y - \zeta/2p$ in a pathological limit ($p \to 0^+$). In the 1D case A has negative parity, so that formally at least supersymmetry renders states of opposite parity degenerate, as Imbo and Sukhatme (1985) state. However this does not escape the controversial questions; $A(0)\Omega_m$ is undefined and $H_m = H$, so that the supersymmetric construction fails to generate a ladder of solutions. The relativistic equations discussed below do allow such a construction since the fine structure terms avoid the pathological limit.

4.2. Klein-Gordon-Coulomb equations

The method parallels § 3. In the 3D case, the Hamiltonian $qA_0 + [(pc)^2 + (m_0c^2)^2]^{1/2}$ with $qA_0 = -\alpha\hbar c/r$ and $\boldsymbol{p} = -\mathrm{i}\hbar\boldsymbol{\partial}$ leads to equation (11) with $N \equiv l(l+1) - \alpha^2$, and with $\Omega \equiv y\Phi$, $y \equiv 2\eta kr \equiv 2\alpha Er/\hbar c$ as in § 3. The 1D case leads to an analogous equation with $N \equiv -\alpha^2$, $\Omega \equiv \Phi$, $y \equiv 2\eta k|x|$—formally the same equation with $l = 0$. We may treat their solutions together. Since $p(p-1) = l(l+1) - \alpha^2$, $p^{(1)} = (1+\sqrt{R})/2$ or $p^{(2)} = (1-\sqrt{R})/2$, where $R = 1 + 4[l(l+1) - \alpha^2]$.

$p^{(1)}$ is the only positive value for $l \neq 0$ and generates the standard ladders of solutions. Successive levels may be removed using a supersymmetric hierarchy of Hamiltonians and hence the eigenvalues of equation (8) and the eigenfunctions of equation (9*b*) where $p_m \equiv p^{(1)} + m$. None of the Hamiltonians H_m with $m > 0$ are of physical interest; the Klein-Gordon-Coulomb system has no supersymmetric degeneracies. For general p, the eigenvalues are given by

$$E(m, p) = m_0c^2(p+m)/[l(l+1) + m^2 + (2m+1)p]^{1/2}.$$

In addition, for $l = 0$, $p^{(2)}$ ($\equiv p^*$) is positive and is associated with a deeply bound and sharply peaked state. The 'ground' states (for p, p^* respectively) have energies given by $E_0(*) \equiv m_0c^2\sqrt{p^{(*)}} = \frac{1}{2}m_0c^2[(1+2\alpha)^{1/2} \pm (1-2\alpha)^{1/2}]$, so that $E_0^* \approx \alpha m_0c^2$. The

two ladders of eigenstates may be constructed as before, giving equations (9) and (10) with $\eta_m^{(*)} = p_m^{(*)} = p^{(*)} + m$. The first few eigenstates of H_0 are (for $p = (1 \pm \sqrt{R})/2$)

$$\Omega_0 = y^p \exp(-\zeta y/2p),$$

$$\Omega_1 = [y^p/2 - \zeta y^{p+1}/(3 \pm R)(5 \pm R)] \exp[-\zeta y/2(p+1)].$$

The excited states $\Omega_m^{(*)}$ are not sharply peaked but have the typical extension of a Bohr radius ($\sim \lambda_c/\alpha$). (The discussion by Spector and Lee (1985), which does not employ supersymmetry, gives several of these results for the 1D case, but confuses the spectra of the two ladders.) The spectrum of the two ladders is given in figure 2.

The 1D case has little affinity with, and so gives little support for, the discussion of Imbo and Sukhatme (1985) for the non-relativistic limit. Parity is not relevant for eigenfunctions with non-integral exponents p, and we have no simple relation as suggested by Loudon (1959) in the non-relativistic case for degenerate, or near degenerate, eigenfunctions; the analytic form of the wavefunction Ω guarantees that Ω and

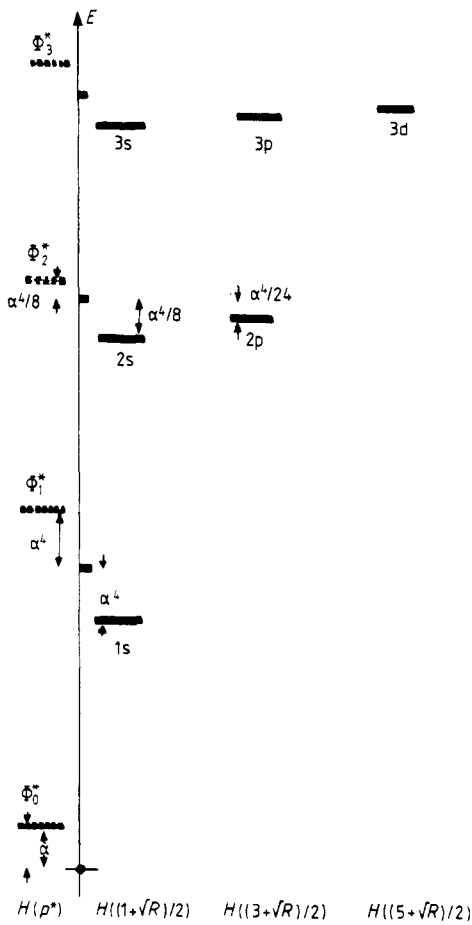

Figure 2. Schematic energy level scheme (not to scale) for the lowest energy solutions of the 3D Klein-Gordon-Coulomb equation. Supersymmetric partner states (solutions of $H'(p)$) are always unphysical, and not depicted here. Solutions of the 1D Klein-Gordon-Coulomb system correspond to the first two columns (i.e. $l = 0$). Solutions of the 1D Dirac-Coulomb system correspond to the second column only. Notation is as for figure 1.

$D\Omega$ match at the origin. $A_0\Omega_m^*$ is non-normalisable, and though $A_0^*\Omega_m$ is normalisable, the Hamiltonian of which it is an eigenstate is unphysical.

5. Solutions of the Dirac–Coulomb systems

5.1. 3D Dirac-Coulomb system

First we relate the Lippmann-Johnson helicity transfer operator to the supersymmetry discussed above. The operators $A^{\pm}$ essentially perform this function, since the degenerate states between which they transform (figure 1) have opposite expectation values λ of Λ, and hence opposite signs for $\langle \boldsymbol{\sigma} \cdot \boldsymbol{L} \rangle$ and $\langle \boldsymbol{\sigma} \cdot \boldsymbol{J} \rangle$. In detail, the general supersymmetric construction (Sukumar 1985b, c) applied to equation (6) gives

$$A(\bar{\kappa}) y \Phi_{n,|\kappa|,-} = (\varepsilon_n - \varepsilon_0)^{1/2} y \Phi_{n-1,|\kappa|,+}$$

$$A^{+}(\bar{\kappa}) y \Phi_{n-1,|\kappa|,+} = (\varepsilon_n - \varepsilon_0)^{1/2} y \Phi_{n,|\kappa|,-}$$

which on rearrangement gives ($\mu = \mathrm{sgn}(\lambda) = \pm 1$)

$$\{1 - (\mu\bar{\kappa}/\eta k)[\partial_r + (\mu\bar{\kappa} + 1)/r]\}\Phi_{n,|\kappa|,\mu} = [1 - (\bar{\kappa}/\eta)^2]^{1/2} \Phi_{n',|\kappa|,-\mu} \tag{12}$$

(the n values being those appropriate to states at a given level) in essential agreement with equation (69) of Biedenharn (1983).

The mass projection operators may be rewritten using equation (12), and also (Martin and Glauber 1958) $c\boldsymbol{\alpha} \cdot \boldsymbol{p} = c\boldsymbol{\alpha} \cdot \hat{\boldsymbol{r}}(p_r + \mathrm{i}\boldsymbol{\sigma} \cdot \boldsymbol{L}/r)$:

$$O_{\pm} = \beta\{E - (\hbar c/\alpha)(\Lambda - K/\hbar)[\partial_r + (\Lambda + 1)/r]\} \pm m_0 c^2.$$

This gives the projected functions the form

$$O_{+}\Phi_{n,|\kappa|,\mu} = (m_0 c^2 + \beta E \mu K/\hbar\bar{\kappa})\Phi_{n,|\kappa|,\mu} + (\beta E/\eta)(\bar{\kappa} + \mu K/\hbar)[(\eta/\bar{\kappa})^2 - 1]^{1/2} \Phi_{n',|\kappa|,-\mu}. \tag{13}$$

For example, the projection of the ground state on the supersymmetric ladder for any $|\kappa|$ gives

$$O_{+}\Phi_{0,|\kappa|,-} = m_0 c^2 (1 - \beta K/\hbar|\kappa|)\Phi_{0,|\kappa|,-}$$

so that $\kappa = -|\kappa|$ for a positive-mass projection to exist. In this case ($\mathrm{sgn}(\lambda) = -1$) $\mathrm{sgn}(\kappa) = -1(+1)$ for the positive- (negative-) mass projections. In general, each projection can be obtained from either choice of $\mathrm{sgn}(\lambda)$. It is convenient to choose $\mathrm{sgn}(\kappa) = \mu \equiv \mathrm{sgn}(\lambda)$ to avoid a tendency—and in the above case, certainty—for cancellation in the first term of equation (13) (Martin and Glauber 1958).

Similarly the additional states may be projected; however, they give non-normalisable functions. For example:

$$O_{+}\Phi_0^* = \beta\{m_0 c^2 (1 - 2\bar{\kappa} - K/\hbar)/[(1+\alpha)^{1/2} - (1-\alpha)^{1/2}] + (\hbar c/\alpha r)(3 - 2\bar{\kappa})(\bar{\kappa} + K/\hbar)\}\Phi_0^*. \tag{14}$$

The normalisation constraints on solutions of the Dirac equation are again that the exponential part vanishes at infinity and that the leading power law exponent be greater than $-\frac{1}{2}$. The function of equation (14) has a leading exponent y^{p^*-1}, and so is non-normalisable, explaining the absence of the corresponding solutions for the Dirac equation.

5.2. 1D Dirac-Coulomb system

The 1D Dirac-Coulomb system is governed by $O_-\Psi = 0$, where now $O_\pm \equiv -i\hbar c\gamma_1 \partial_x + \gamma_0(E + \alpha\hbar c/|x|) \pm m_0c^2$. Inserting the gamma matrices gives two sets of coupled first-order radial equations, and it is readily checked that no nodeless solutions of the form $x^p \exp(-q|x|)$ exist in any scalar basis at finite energy. The 'direct' supersymmetric approach then fails, at least in its simplest form. Indeed, no general solution of this equation has been traced despite its obvious physical interest.

However the analogue of Kramers' equation ($O_-O_+\Psi = 0$) is just that for the 1D Klein-Gordon-Coulomb system. Hence we may project the solutions of § 4.2 by O_+ to obtain solutions of the 1D Dirac-Coulomb system. The states corresponding to p^* are non-normalisable, and so unphysical (as in § 5.1), but the states associated with $p = \frac{1}{2}(1+\sqrt{R})$ give rise to valid solutions of the form $O_+\Omega_m$ with the same spectrum $(E(m, (1+\sqrt{R})/2))$ as for these solutions of the 1D Klein-Gordon-Coulomb system. For example, the $l = 0$ ground state has the form

$$O_+\Omega_0 \propto \{-2\alpha i\gamma_1[(1+\sqrt{R})/2y - \zeta/(1+\sqrt{R})] + \gamma_0(1+2\alpha^2\zeta/y) + m_0c^2/E_0\}y^{(1+\sqrt{R})/2} \times \exp[-\zeta y/(1+\sqrt{R})].$$

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