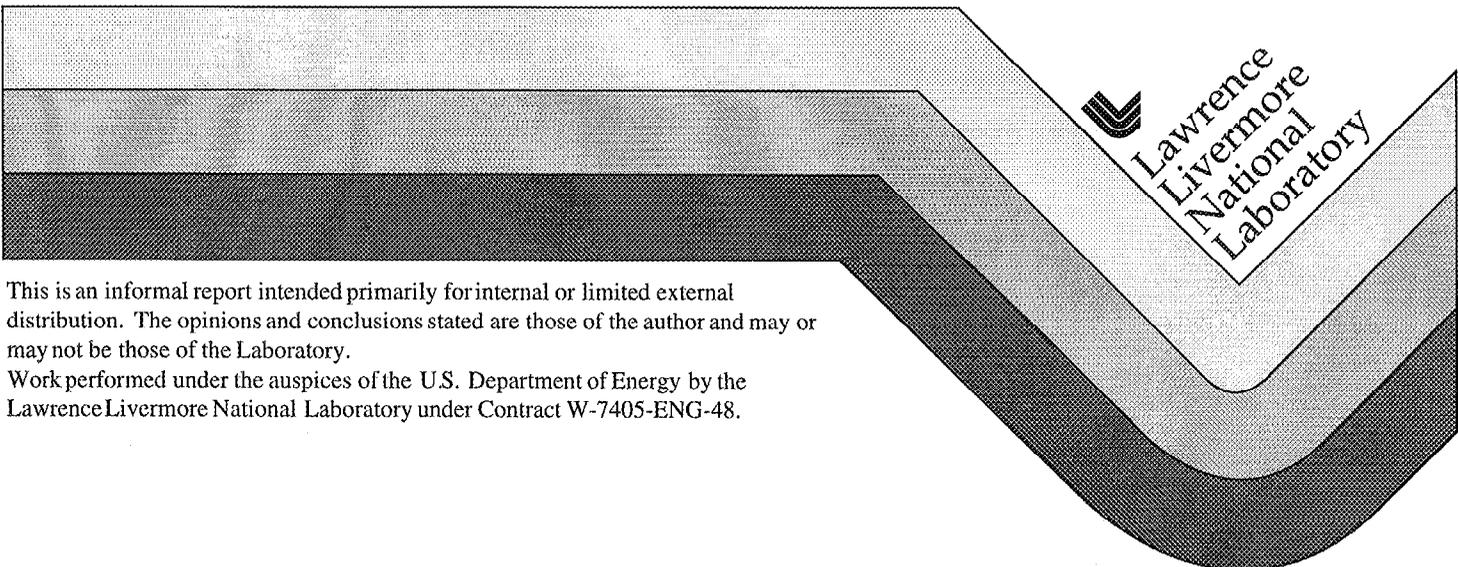


# Use of the Lorentz-operator in Relativistic Quantum Mechanics to Guarantee a Single-energy Root

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Use of the Lorentz-operator in relativistic quantum  
mechanics to guarantee a single-energy root

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The Lorentz-operator form of relativistic quantum  
mechanics, with relativistic wave equation 
$$\hat{H} \frac{\partial \psi}{\partial t} = (mc^2 \gamma + e\Phi) \psi$$

is implemented to guarantee a single-energy root. The  
Lorentz factor as modified by Pauli's *ansatz* is given by

$$\gamma = \sqrt{1 + \frac{[\vec{\sigma} \cdot (\hat{h} \vec{\nabla} + \frac{e}{c} \vec{A})]^2}{m^2 c^2}},$$
 such that the theory is appropriate

for electrons. Magnetic fine structure in the Lorentz  
relativistic wave equation emerges on the use of an  
appropriate operator form of the Lienard-Wiechert four-  
potential  $(\Phi, \vec{A})$  from electromagnetic theory. Although  
computationally more intensive the advantage of the theory  
is the elimination of the negative-root of the energy and an  
interpretation of the wave function based on a one-  
particle, positive definite probability density like that  
of nonrelativistic quantum mechanics.

## I. Introduction

The relativistic wave equation which is inferred directly from the special theory of relativity is well known to be,

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi \quad (1a)$$

$$H = mc^2 \gamma + e\Phi, \quad (1b)$$

where  $\gamma$  is the Lorentz factor,

$$\gamma = \sqrt{1 + \frac{p^2}{m^2 c^2}}, \quad (2)$$

and in Eq. (2)  $p^2 \rightarrow -\hbar^2 \nabla^2$ . The square-root operation is sometimes regarded as undefined; however a square-root operation of the form given by Eq. (2) has been used for example in optical physics [1]. The operation is performed by expanding the square root, even outside its radius of convergence, successively operating on an eigenfunction of the Laplacian term by term, and then re-collapsing the series back into the compact form of the square root. In the above example the wave function is expanded in a Fourier series and the Lorentz operator is evaluated to give simply,

$$\gamma = \sqrt{1 + \frac{\hbar^2 k^2}{m^2 c^2}} \quad (3)$$

Historically Schroedinger derived his nonrelativistic wave equation by expanding the square root to first order in the Laplacian. One observes however that such a truncated expansion could not be expected to be reliable for an S-state for motion in an attractive Coulomb field, even for small nuclear charge Z, because for small enough radius the motion must become ultra-relativistic ( $p \gg mc$ ). Thus the so-called nonrelativistic limit is not well defined for S-states. The success of nonrelativistic theory for small-Z S-states depends on the happenstance that on average the electron spends a preponderance of its time far enough from the nucleus such that  $p \ll mc$ .

There are situations however in which this on-average distant motion does not obtain. For example the Klein-Gordon equation, in which the operation of the Laplacian is linearized at the cost of casting relativistic quantum theory in a form with a double-root energy,

$$\left( i \hbar \frac{\partial}{\partial t} - e\Phi \right)^2 \chi = (m^2 c^4 + c^2 \nabla^2) \chi \quad (4)$$

actually has two normalizable 1s states, one of which has a binding

energy nearly equal to  $mc^2$  (Fig. 1) and is identified with the Schroedinger 1s wave function irregular at the origin [2], while the other is identified with the Schroedinger 1s wave function regular at the origin. This state has not attracted interest because it is not physically realizable in an atom, where the source of the Coulomb potential is not a point, such that it can be argued [3] that the only physically interpretable solution of the Klein-Gordon equation is the one which agrees with the regular Schroedinger solution in the "nonrelativistic limit." Such arguments are not appropriate however when there really is a point source of attraction such as a positron [2]. The overcompleteness of the S-state basis in Klein-Gordon theory suggests a pathology possibly related to its quadratic form; however in practice this overcompleteness is not of serious consequence since the vast energy difference between the two 1s states causes them to be nearly orthogonal [2].

The resolution by Dirac of the double-root ambiguity in the energy is of course well known and forms the basis for the practical application of this form of relativistic quantum theory, namely that the collapse of the atom by spontaneous radiative decay from

positive-energy to negative-energy states is averted by filling the negative energy-states with a "sea" of electrons ("particles"), a vacancy in which signifies a positron ("hole"). It is curious that although spontaneous radiative transitions are allowed to *unfilled* negative-energy states, the motion in the negative-energy regime is repulsive and not attractive through the term  $-2Ee\Phi$  in Eq. (4) (and similarly in the Dirac equation), which causes the motion to be attractive for  $e\Phi < 0, E > 0$  but repulsive for  $e\Phi < 0, E < 0$ . Thus the hydrogenic spectrum lies wholly in the  $e\Phi < 0, E > 0$  regime and in the  $e\Phi < 0, E < 0$  regime there are no bound states but only the negative-energy continuum which lies  $-mc^2$  below  $E = 0$  (Fig. 2). The mirror image of this spectrum exists for positive potentials (Fig. 3), for which the motion is repulsive in the regime  $e\Phi > 0, E > 0$  but attractive in the regime  $e\Phi > 0, E < 0$  such that for example a positron moving in the field of a proton will have a hydrogenic spectrum of bound states lying above  $-mc^2$  in the  $e\Phi > 0, E < 0$  regime, to which it can make spontaneous radiative transitions unless these levels are already filled with a "sea" of positrons.

To this author it seems intolerable that the simple repulsive motion of two particles having the same charge cannot be understood without invoking Dirac's *ansatz*. It seems clear that neither scenario will be predicted by Eq. (1), which is single-valued in its energy spectrum. Thus we are motivated to formulate relativistic quantum mechanics as a single-spectral, single-particle theory with positive-definite probability density.

An interpretation of matter-antimatter annihilation reactions which is radically different from Dirac's is immediately suggested by classical relativistic theory [4], in which a particle with angular momentum  $L < e^2/c$  in an attractive Coulomb field falls to the center of attraction even in absence of the electromagnetic field. In relativistic quantum theory the uncertainty principle guarantees that the motion of such a collapsed state will stabilize in a small volume about the center of attraction, and indeed the ultra-relativistically bound state predicted by Klein-Gordon theory (Fig. 1) confirms this expectation [2]. The binding energy of this state is less than  $2mc^2$  by about 0.4 % (Fig. 1), which is well outside the error bars of existing experiments which seem to confirm that

precisely  $2mc^2$  of energy is radiated by two photons in annihilation, as predicted by Dirac theory. However, in a single-root theory such as that of Eq. (1), in which a negative-energy regime and a many-particle interpretation of the wave function seem not to be available, one would have to infer that annihilation would be represented by two-photon decay to an ultra-relativistically bound state whose binding is  $2mc^2$  within the error bars of existing precision experiments. Also single-root theory suggests that annihilation reactions may produce two photons and a nearly massless neutrino, which provides a new degree of freedom to experimental investigations.

These particle-physics implications of single-root theory are not of that much interest however in relativistic quantum chemistry, except for the concern of what constitutes a complete set of states and how these states are accurately calculated for an atom or molecule. These are the same concerns however in conventional Dirac-theory calculations, in which for example a complete set of states in a perturbative calculation comprises both the positive-

and negative-energy states. Thus the practical advantage of single-root theory appears to be conceptual rather than computational: it provides a single-particle interpretation with positive definite probability density in analogy to nonrelativistic quantum theory.

## II. Theory

First we modify the Hamiltonian by using Pauli's *ansatz* in

Eq. (2)  $\vec{p} - \frac{e\vec{A}}{c} \rightarrow \sigma \left( \vec{p} - \frac{e\vec{A}}{c} \right)$  such that the Hamiltonian of Eq. (1)

becomes,

$$H = \sqrt{m^2 c^4 + c^2 \left[ \sigma \cdot \left( \vec{p} - \frac{e\vec{A}}{c} \right) \right]^2} + e\Phi, \quad (5)$$

is now appropriate for an electron. The second term under the square root can be written in the more familiar form,

$$\left[ \sigma \cdot \left( \vec{p} - \frac{e\vec{A}}{c} \right) \right]^2 = \left( \vec{p} - \frac{e\vec{A}}{c} \right)^2 - \frac{e\hbar}{c} \sigma \cdot (\nabla \times \vec{A}), \quad (6)$$

such that expansion of the square root immediately gives the Pauli Hamiltonian to first order in the operator. Now how is the operation determined by the square root in Eq. (5) defined? We can infer its definition by dropping the scalar potential, transposing the right-hand term to the left side in Eq. (1a), such that,

$$\left( i\hbar \frac{\partial}{\partial t} - \sqrt{m^2 c^4 + c^2 [\vec{\sigma} \cdot (\vec{p} - \frac{e}{c} \vec{A})]^2} \right) \psi = 0 \quad (7a)$$

operating on Eq. (7a) from the left with,

$$i\hbar \frac{\partial}{\partial t} + \sqrt{m^2 c^4 + c^2 [\vec{\sigma} \cdot (\vec{p} - \frac{e}{c} \vec{A})]^2} \quad (7b)$$

and using Eq. (6) to obtain,

$$\left\{ \hbar^2 \frac{\partial^2}{\partial t^2} + m^2 c^4 + c^2 \left[ (\vec{p} - \frac{e}{c} \vec{A})^2 - \frac{e\hbar}{c} \vec{\sigma} \cdot (\vec{\nabla} \times \vec{A}) \right] \right\} \psi = 0 \quad (8)$$

This equation is identical to the Dirac equation when  $\Phi = 0$  ; thus its positive-energy solutions are also solutions to the Lorentz relativistic wave equation (LRWE) [Eq. (1)] when  $\Phi = 0$  and form a complete set in this subspace which can be used to expand the wave function of the LRWE when  $\Phi$  is not zero. We can also infer from Eq. (8) that the LRWE satisfies the correct energy-momentum relation for a free particle and is Lorentz covariant. From Eq. (1) we have already inferred that the LRWE form of relativistic quantum theory satisfies the demand which motivated the present work: that of a theory with a single-particle, positive definite probability density interpretation. Thus it is close to Dirac theory, but without

the negative root to the energy, such that the third demand above, which goes back to the original formulation of Dirac but was later abandoned by him because of the presence of the negative-energy root, can be satisfied.

Although there are no obvious approximations as yet, still the LRWE appears not to describe the magnetic fine structure of the atom. This omission is only apparent however when we realize that a relativistic matter theory should be used in conjunction with a relativistically invariant form of the electromagnetic potentials. This means that one should use, not just the scalar potential  $\Phi$ , but the four-vector potential  $(\Phi, \vec{A})$ , which for the Coulomb field is just the Lenard-Wiechert four-potential [5]. In the moving frame of the electron the scalar and vector components of this potential are,

$$\Phi = -\frac{Ze}{r} \quad (9a)$$

$$\vec{A} = \frac{Ze}{r} \frac{\vec{v}}{c}, \quad (9b)$$

where we have neglected retardation over the scale of the atom. In order to take the vector component over into quantum mechanics, it must be in an appropriate operator form. We write the *ansatz*,

$$\vec{A} = -i \frac{Ze\hbar}{2mc} \left[ \frac{1}{r} \vec{\nabla} - \vec{\nabla} \left( \frac{1}{r} \right) \right], \quad (10)$$

where we have used the standard operator replacement  $\vec{v} = \frac{-i\hbar}{m} \vec{\nabla}$  and a symmetrization which insures the antisymmetry of the magnetic field  $\vec{\nabla} \times \vec{A} = -\vec{A} \times \vec{\nabla}$  associated with the electron's motion.

Before Dirac's equation the spin-orbit interaction had been derived [6] from the Pauli term in Eq. (6), or more precisely from the expanded square root of Eq. (5), where to first-order in the operator, the Pauli interaction is,

$$H_p = -\frac{e\hbar}{2mc} \vec{\sigma} \cdot (\vec{\nabla} \times \vec{A}) \quad (11)$$

using classical arguments, namely that in a frame moving with the electron the magnetic field and energy associated with the orbital motion is,

$$\vec{\nabla} \times \vec{A} = -c^{-1} \vec{v} \times \vec{E} = -\frac{1}{c} \frac{1}{r} \frac{d\Phi}{dr} (\vec{r} \times \vec{v}) \quad (12a)$$

$$H_{so} = \frac{e\hbar}{2m^2 c^2} \frac{1}{r} \frac{d\Phi}{dr} \vec{\sigma} \cdot \vec{L}_c + \frac{1}{2} \vec{\sigma} \cdot \hbar \omega_T \quad (12b)$$

where  $\vec{L}_c = m(\vec{r} \times \vec{v})$ . Eq. (12a) is obtained from the curl of Eq. (9b); its substitution into Eq. (11) gives the first term on the right side of Eq. (12b). The second term on the right side of Eq. (12b) is the Thomas precession [6], whose origin is the rotation of the frame moving

with the electron about the nucleus. It contributes a counter term which is minus one-half of the first term, so that the classically derived spin-orbit interaction agrees with Dirac theory.

Although these classical arguments eventually lead to the correct form of the spin-orbit interaction, the passage to the operator form of Eqs. (12), in which  $\vec{r} \times \vec{v} \rightarrow -\frac{i\hbar}{m} \vec{r} \times \vec{\nabla} = \frac{\hbar}{m} \vec{L}$ , is clearly flawed because the importance of the order of the operators in the product is ignored. On the other hand the symmetrized form of the vector potential given by Eq. (10) is simply a weighted average of the two possible ordered products, with relative weights chosen to give simultaneously the correct spin-orbit interaction and the correct antisymmetry of the *operator* magnetic field associated with the electron's orbital motion. Obviously the rule  $\vec{\nabla} \times \vec{A} = -\vec{A} \times \vec{\nabla}$  must be observed in any operator field one writes since the Pauli Hamiltonian itself [see Eq. (6)] depends on the cancellation of operators  $\vec{\nabla} \times \vec{A}$  and  $\vec{A} \times \vec{\nabla}$  in which the gradient operates in both cases on the wave function and not on the vector field. Eq. (10) leads to the correct spin-orbit interaction without invoking Thomas

precession; thus it is possible that the physics of the counter term which Thomas precession contributes is also described, although in a way which is not clear at present, by using the symmetrized operator in the Hamiltonian. Inevitably it contributes terms in addition to the correct spin-orbit interaction, which as it turns out are important only close to the origin or for S-states, as we shall see. Thus for angular momentum  $L > 0$ , for which the expansion of the square-root can be reliably made in the so-called nonrelativistic limit, the LRWE with four-potential is in exact agreement with Dirac theory. Obviously however this derivation of the magnetic fine structure is heuristic and not entirely satisfactory because it finds an operator form from the classically derived four-potential  $(\Phi, \vec{A})$ , which is fine when the vector component is ignored except for externally applied fields, as in nonrelativistic theory. A more satisfactory procedure would be to derive the four-potential using a quantum mechanical operator form of Maxwell's equations for the potentials, as in quantum electrodynamics (QED). In a complete theory then quantum Maxwell theory would be used both for the static four-potential and for the dynamic four-potential which

causes QED corrections to the motion.

Dirac's treatment does not require the explicit use of the static four-potential to describe magnetic fine structure; however Dirac's equation can be cast in the form which would be precisely

a statement of the relativistic invariance of the square of the four

momentum operator  $(\frac{i\hbar}{c} \frac{\partial}{\partial t} - e\Phi, \vec{\sigma} \cdot [\vec{p} - \frac{e}{c} \vec{A}])$  if the noncommutivity of the scalar and vector components of the four momentum were

ignored. This form of the Dirac equation is [7],

$$[\frac{i\hbar}{c} \frac{\partial}{\partial t} - e\Phi - \vec{\sigma} \cdot (\vec{p} - \frac{e}{c} \vec{A})][\frac{i\hbar}{c} \frac{\partial}{\partial t} + \vec{\sigma} \cdot (\vec{p} - \frac{e}{c} \vec{A})] \psi = m^2 c^2 \psi, \quad (13)$$

where magnetic fine structure emerges from the noncommutivity of the second term in the first square bracket and the first term in the second square bracket. On the other hand the Klein-Gordon equation is precisely a statement of the relativistic invariance of

the square of the four momentum  $(\frac{i\hbar}{c} \frac{\partial}{\partial t} - e\Phi, \vec{p} - \frac{e}{c} \vec{A})$ , namely,

$$[\frac{(i\hbar}{c} \frac{\partial}{\partial t} - e\Phi)^2 - (\vec{p} - \frac{e}{c} \vec{A})^2] \chi = m^2 c^2 \chi \quad (14)$$

Finally, returning to the LRWE and using Eq. (10) and its curl in Eq. (6), one has,

$$[\vec{\sigma} \cdot (c \vec{p} - e \vec{A})]^2 = -\hbar^2 \left( v \vec{\nabla} + \frac{e}{2mc} \vec{E} \right)^2 + \frac{e\hbar^2}{2m} \frac{d\Phi}{dr} \frac{\vec{\sigma} \cdot \vec{L}}{r} \quad (15a)$$

$$v = c + \frac{e}{2mc} \Phi \quad (15b)$$

$$\vec{E} = -\vec{\nabla} \Phi \quad (15c)$$

$$\vec{L} = -i \vec{r} \times \vec{\nabla} \quad (15d)$$

One notes that on expanding the square root in Eq. (5) and using Eq. (15a) the correct spin-orbit interaction emerges,

$$H_{so} = \frac{e\hbar^2}{4m^2 c^2} \frac{d\Phi}{dr} \frac{\vec{\sigma} \cdot \vec{L}}{r} \quad (16)$$

### III. Ultra-relativistic motion

The LRWE [Eq. (1)] insures that the energy is single-valued; however one would expect for there to be a counterpart to the negative-energy continuum of Dirac theory since otherwise, when the electron couples to the quantum electromagnetic field, the LRWE would be unable to describe two-photon radiative decay, with energy

loss of  $mc^2$  per electron mass, which is characteristic of the Dirac spectrum when there is a hole at  $-mc^2$ . Just as in Dirac theory it is necessary to resolve this issue before one can use the theory in practical atomic physics applications.

Remarkably the LRWE spectrum is divided into two subregions, which are characterized by the range of values of the velocity given by Eq. (15b), which can be regarded as a renormalized speed of light whose origin is the operator vector potential [Eq. (10)]. Recall that the curl of the vector potential is the magnetic field which gives the correct spin-orbit interaction [Eq. (16)] when substituted into the Pauli interaction in the Hamiltonian; similarly when the vector potential is used in the kinetic momentum  $\vec{p} - \frac{e}{c}\vec{A}$ , it leads to the renormalized speed of light.

The critical values of the renormalized speed are  $v = 0$  at an electron radius  $r = e^2/2mc^2$  (for a unit-strength Coulomb potential), which is roughly the radius of the nucleus, and  $v \rightarrow -\infty$  as  $r \rightarrow 0$ .

Remarkably the wave function vanishes at  $v = 0$ ,  $r = e^2/2mc^2$  and diverges as  $r^{-1}$  at  $v \rightarrow -\infty$ ,  $r \rightarrow 0$ . This suggests an identification of

the subregion  $0 < r < e^2/2mc^2$ , in which particles can be sucked in near the origin, with the negative-energy continuum of Dirac theory, in which similarly the electron coupled to the electromagnetic field can cascade to oblivion as  $E \rightarrow -\infty$ . It is also tempting to compare the negative range of the speed  $v$  in the "nuclear" sphere, which implies a clock running backwards, with the Feynman boundary conditions for negative-energy states in which negative-energy waves propagate backwards in time [8]. In any event the theory should be extended to include the point-particle source of the Coulomb field, so that the possibility exists that source recoil will soften the potential enough to give a physically interpretable wave function at the origin.

Alternatively one must use a device similar to that of Dirac which consists of filling up the "nuclear" levels to a point such that particle mass is conserved. Thus the LRWE seems to suffer a fate very analogous to Dirac theory, which similarly points toward a many-body resolution; however the LRWE suggests a physical origin for these difficulties and, intriguingly, predicts a separation of the

motion into two subregions of space and energy, one nuclear for the renormalized speed in the regime  $-\infty < v < 0$  and the other atomic in the regime  $0 < v < c$ .

In what follows we support the foregoing remarks by examining the motion when the electron is close to the center of force. We assume that the second term under the square root sign in Eq. (5) dominates the first term. This is known as the ultra-relativistic regime, where  $p \gg mc$  [9,10]. On making the steady assumption  $i\hbar \frac{\partial}{\partial t} \rightarrow E$ , we obtain,

$$c \vec{\sigma} \cdot \left( \vec{p} - \frac{e}{c} \vec{A} \right) \psi + e\Phi \psi = E \psi \quad (17)$$

This equation is close in form to Dirac's equation, so that we can use standard methods in its analysis. First we expand the wave function,

$$\psi = g_{\kappa} \chi_{\kappa\mu} + i g_{-\kappa} \chi_{-\kappa\mu} \quad (18)$$

where  $g_{\kappa}$  is the radial wave function and  $\chi_{\kappa\mu}$  are the two-component spinors with the well known properties,

$$\vec{\sigma} \cdot \vec{L} \chi_{\kappa\mu} = -(\kappa + 1) \chi_{\kappa\mu} \quad (19a)$$

$$\hat{\sigma} \cdot \hat{r} \chi_{\kappa\mu} = -\chi_{-\kappa\mu} \quad (19b)$$

Substituting Eq. (18) into Eq. (17) and using Eqs. (19), (9a), and (10) and the identity,

$$\vec{\sigma} \cdot \vec{\nabla} = \hat{\sigma} \cdot \hat{r} \left( \frac{\partial}{\partial r} - \frac{\vec{\sigma} \cdot \vec{L}}{r} \right) \quad (20)$$

we derive the pair of coupled radial equations,

$$\left[ \hbar v \left( \frac{d}{dr} + \frac{\kappa + 1}{r} \right) - \frac{e\hbar}{2mc} \Phi' \right] g_{\kappa} + (e\Phi - E) g_{-\kappa} = 0 \quad (21a)$$

$$\left[ \hbar v \left( \frac{d}{dr} - \frac{\kappa - 1}{r} \right) - \frac{e\hbar}{2mc} \Phi' \right] g_{-\kappa} - (e\Phi - E) g_{\kappa} = 0 \quad (21b)$$

where the prime denotes derivative with respect to  $r$  and  $v$  is given by Eq. (15b). Eliminating Eq. (21b) in favor of Eq. (21a) one has,

$$\begin{aligned} & \left[ \frac{d^2}{dr^2} + \left( \frac{2}{r} - \frac{e\Phi'}{mcv} \right) \frac{d}{dr} - \frac{\kappa(\kappa+1)}{r^2} - \frac{e\Phi'}{mcv r} + \frac{(e\Phi')^2}{2mcv} \left( \frac{1}{2mcv} - \frac{1}{E - e\Phi} \right) - \frac{e\Phi''}{2mcv} + \right. \\ & \left. + \left( \frac{v'}{v} + \frac{e\Phi'}{E - e\Phi} \right) \left( \frac{d}{dr} + \frac{\kappa+1}{r} \right) + \frac{(e\Phi - E)^2}{\hbar^2 v^2} \right] g_{\kappa} = 0 \end{aligned} \quad (22)$$

First a few general remarks concerning Eq. (22) are in order. Two of the terms,  $-e\Phi'/mcv r$  and  $-e\Phi''/2mcv$ , cancel. If the vector component of the four-potential [Eq. (10)] is ignored, Dirac's

equation is recovered for small  $r$ ,

$$\left(\frac{d^2}{dr^2} + \frac{3}{r} \frac{d}{dr} - \frac{\kappa^2 - 1 - \alpha^2}{r^2}\right)g_\kappa = 0 \quad (23)$$

whose solution regular at the origin is,

$$g_\kappa = r^{\sqrt{\kappa^2 - \alpha^2} - 1} \quad (24)$$

where  $\alpha$  is the fine structure constant. If the vector component and the Dirac-like term [next to the last term on the left side of Eq. (22)] are ignored, the Klein-Gordon equation is recovered for small  $r$ ,

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\kappa(\kappa+1) - \alpha^2}{r^2}\right)g_\kappa = 0 \quad (25)$$

*both* of whose solutions for  $s$  states ( $\kappa = -1$ ) are regular at the origin [2], as discussed earlier,

$$g_\kappa = r^{-\frac{1}{2} \pm \frac{1}{2} \sqrt{1 + 4(\kappa(\kappa+1) - \alpha^2)}} \quad (26)$$

Finally close to  $r = 0$  (for  $\kappa = -1$ ) Eq (22) becomes,

$$\left(\frac{d^2}{dr^2} + \frac{4}{r} \frac{d}{dr} + \frac{2}{r^2}\right)g_\kappa = 0 \quad (27)$$

whose least singular solution is  $r^{-1}$ . Then remarkably a natural boundary is found at  $r = Ze^2/2mc^2$ , where  $v = 0$  and both solutions

vanish. The solutions near this boundary are given by,

$$g_{\kappa} = (2mc^2 r - Ze^2)^{1 \pm i\sqrt{f}} \quad (28a)$$

$$f = \frac{Z^2 e^4}{h^2 m^2 c^6} \left( mc^2 + \frac{E}{2} \right)^2 \quad (28b)$$

Clearly the present theory makes sense at these small distances only if the center of force really is a point source ( $Z = 1$ ). Thus the radius of the boundary is one-half the classical electron radius or  $r = r_0/2$  where  $r_0 = e^2/mc^2$ , which is the order of the nuclear radius. As discussed earlier this result suggests that the negative energy branch of Dirac theory, which is filled with electrons whose energies range from  $-\infty$  to  $-mc^2$  to avert the collapse of the atom, has its counterpart here in states which are localized in a volume about the size of the nucleus. The  $r^{-1}$  behavior at the origin likely reflects the shortcomings of the physical model, namely the assumption of a recoilless point source.

#### IV. Summary and Conclusions

The Lorentz relativistic wave equation (LRWE) has been used to guarantee a single-valued spectrum, positive-definite probability density, and single-particle interpretation of the wave function. Atomic fine structure depends on the use of a relativistically invariant form of the electromagnetic potential, which we take to be a physically appropriate operator form of the Lienard-Wiechert four-potential  $(\Phi, \vec{A})$ . This procedure gives the correct spin-orbit interaction when the curl of the vector component is used to evaluate the Pauli magnetic moment term in the Hamiltonian. The vector component also contributes to the kinetic momentum of the electron in a manner which causes the wave function to vanish on the surface of a sphere of radius  $e^2/2mc^2$  and to diverge as  $r^{-1}$  at the origin. This result suggests a many-body resolution, either explicitly by treating the dynamics of the point source of the Coulomb field or implicitly, as in Dirac theory, by filling up the levels from  $-\infty < E < -mc^2$ , such that a two-photon radiative transition to a hole at  $-mc^2$  represents positron-electron

annihilation. The former procedure is the more fundamental and the point source would be considered to be a positron. Then a critical test of this form of relativistic quantum theory is the existence of of an untra-relativistically bound state in the two-particle spectrum (Fig. 1) such that a two-photon radiative transition will give up an energy of  $2mc^2$  within the error bars of existing experiments.

The latter procedure however is the easier to implement, and we illustrate how the Dirac *ansatz* for filling up the levels in the regime  $-\infty < E < -mc^2$  might work in practice. We know quite generally that the number of quantum levels which can be confined to a small box is sparse, even in the presence of a strong attractive potential. Therefore as an exercise we solve Eq. (22) in the regime  $0 < r < \alpha^2 a_0$  (where  $\alpha$  is the fine structure constant and  $a_0$  is the bohr radius) by finding an energy at which the wave function vanishes at the boundary  $\alpha^2 a_0/2$ , according to Eq. (28a), for a cut off at the origin which is chosen to be small compared to  $\alpha^2 a_0/2$ . The result is shown in Fig. 4, where the energy of the level is indeed

close to  $-mc^2$ , which is the highest occupied negative-energy orbital of Dirac theory. Thus the single level can be saturated by two paired electrons (provided four-potential attraction overcomes their mutual repulsion). The next available level would be expected to lie in the atomic region where  $r > \alpha^2 a_0/2$ , and the familiar S-state cusp behavior close to the nuclear region (i. e. close to  $\alpha^2 a_0/2$ ) would be expected eventually to emerge with increasing  $r$ .

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## Figure Captions

Figure 1. Klein-Gordon spectrum for the relative motion of positronium; the center-of-mass motion is separable if it is assumed to be nonrelativistic.

Figure 2. Dirac spectrum for a negative Coulomb potential  $e\Phi < 0$ , with attraction and binding for  $E > 0$  and repulsion and nonbinding for  $E < 0$ .

Figure 3. Dirac spectrum for a positive Coulomb potential  $e\Phi > 0$ , with repulsion and nonbinding for  $E > 0$  and attraction and binding for  $E < 0$ .

Figure 4. Example of Dirac-like *ansatz* used to fill up the Lorentz relativistic wave equation (LRWE) spectral subregion in the regime  $-\infty < E < -mc^2$ . The plot shows the wave function versus radial distance for a cut off at the origin of  $0.0195 \alpha^2 a_0$  (where  $\alpha$  is the fine structure constant and  $a_0$  the bohr radius) and boundary condition that the wave function vanish at  $\alpha^2 a_0/2$ . The LRWE is satisfied for an energy of  $-0.804022490267 mc^2$ . The number of significant figures shows the sensitivity to the boundary condition.

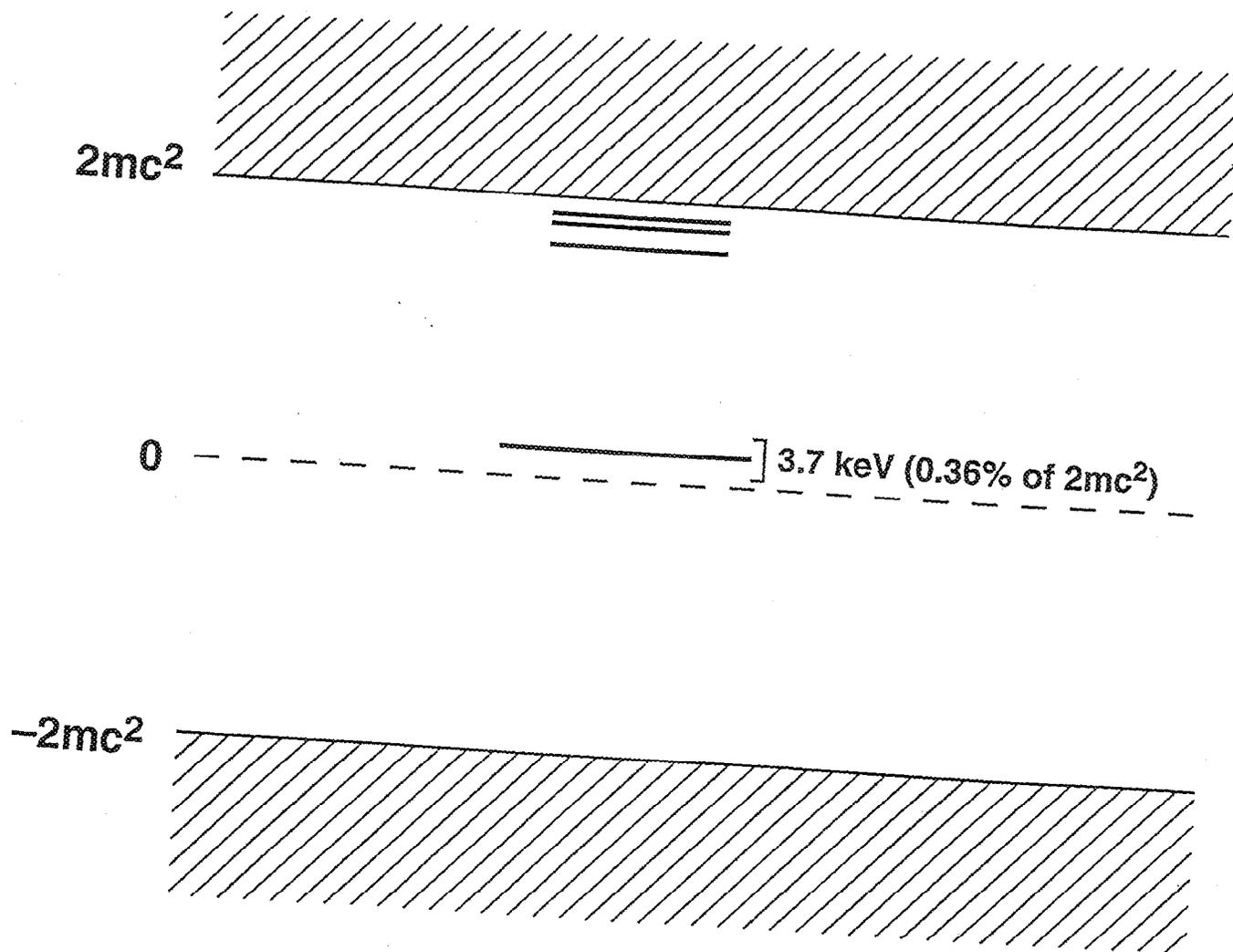


Figure 1. Klein-Gordon spectrum for the relative motion of positronium; the center-of-mass motion is separable if it is assumed to be nonrelativistic.

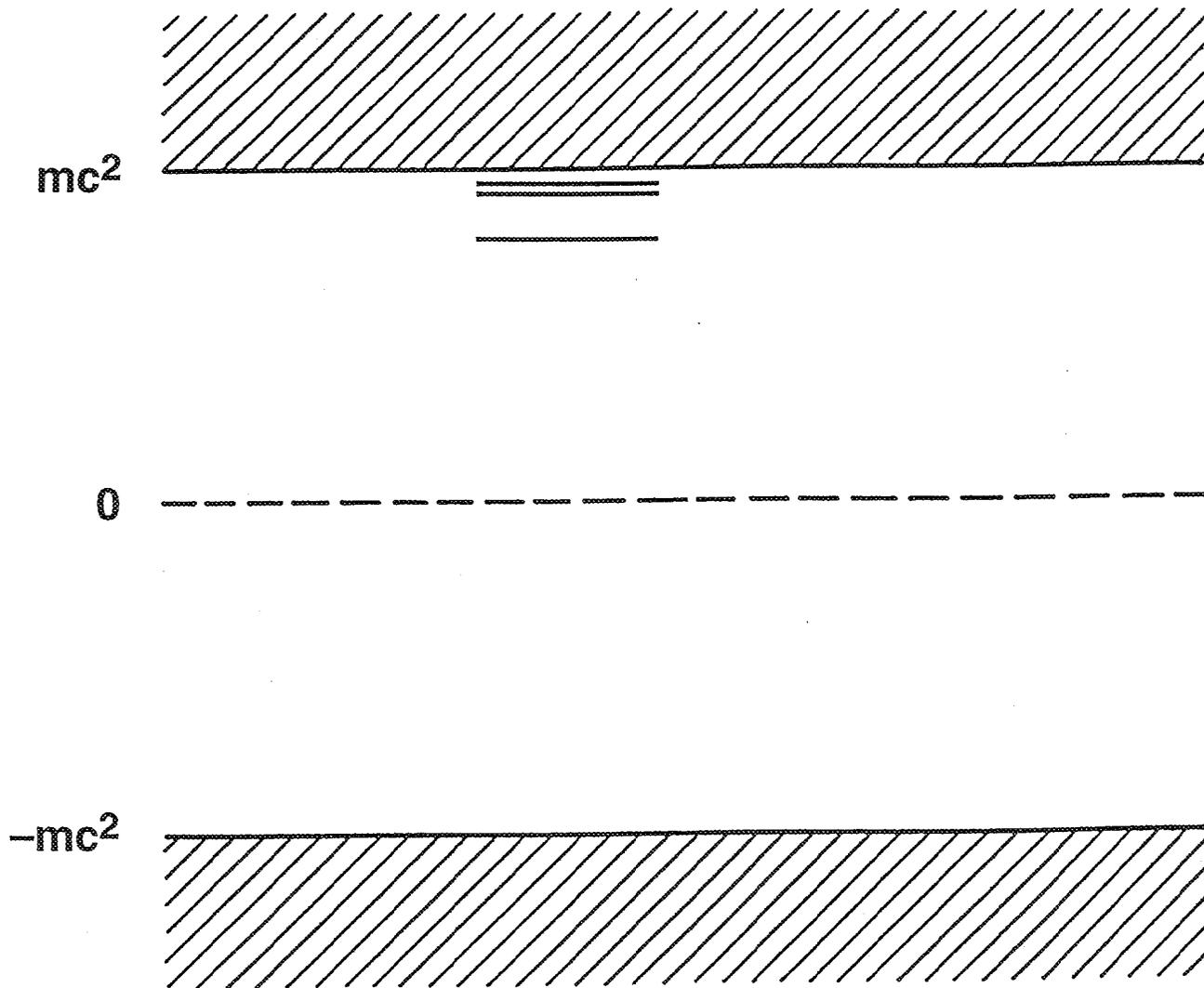


Figure 2. Dirac spectrum for a negative Coulomb potential  $e\Phi < 0$ , with repulsion and nonbinding for  $E < 0$  and attraction and binding for  $E > 0$ .

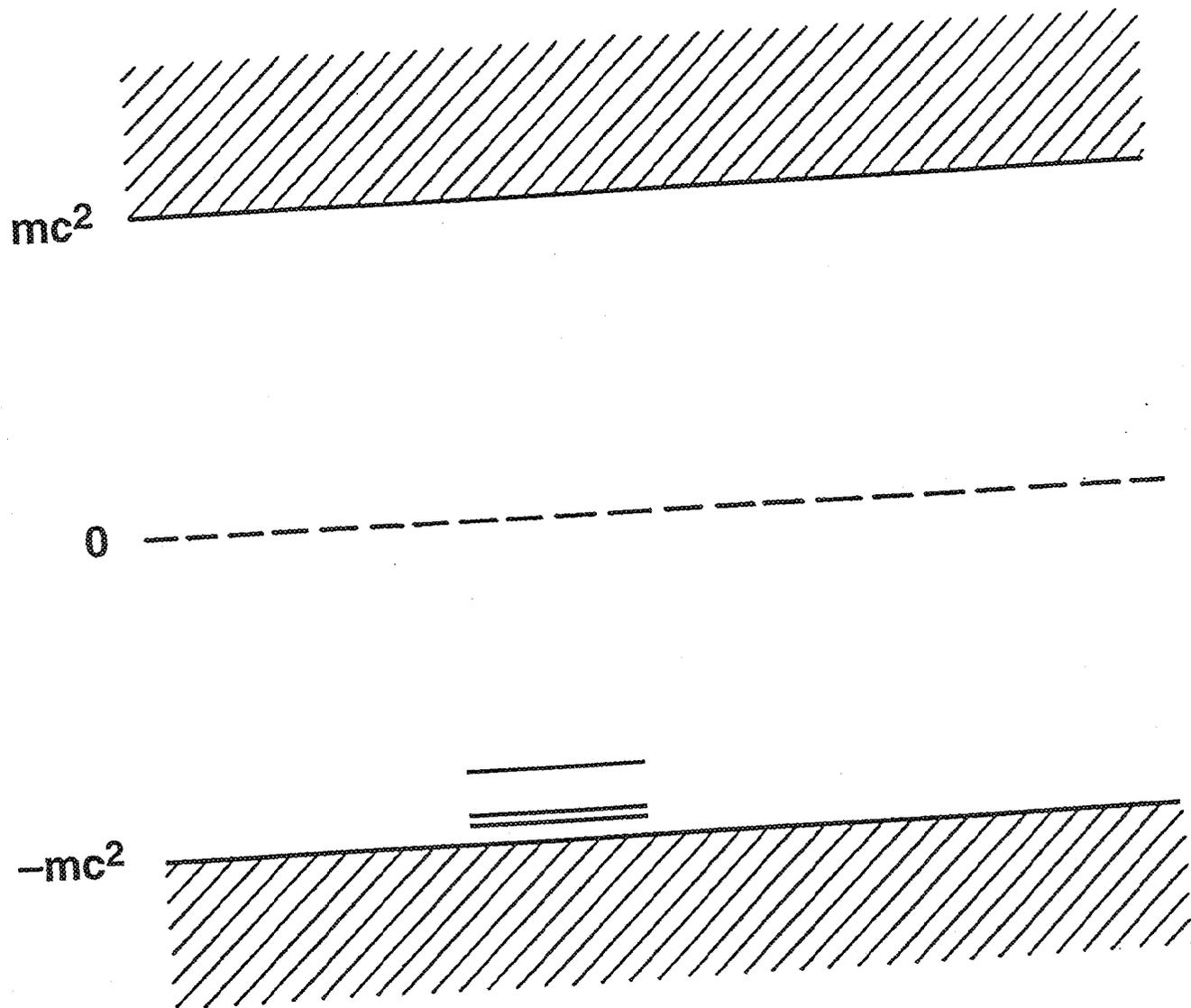


Figure 3. Bizarre aspect of double-energy theory: the mirror image of the Dirac spectrum for a negative Coulomb potential  $e\Phi < 0$  is the Dirac spectrum for a positive Coulomb potential  $e\Phi > 0$ , with repulsion and nonbinding for  $E > 0$  and attraction and binding for  $E < 0$ .

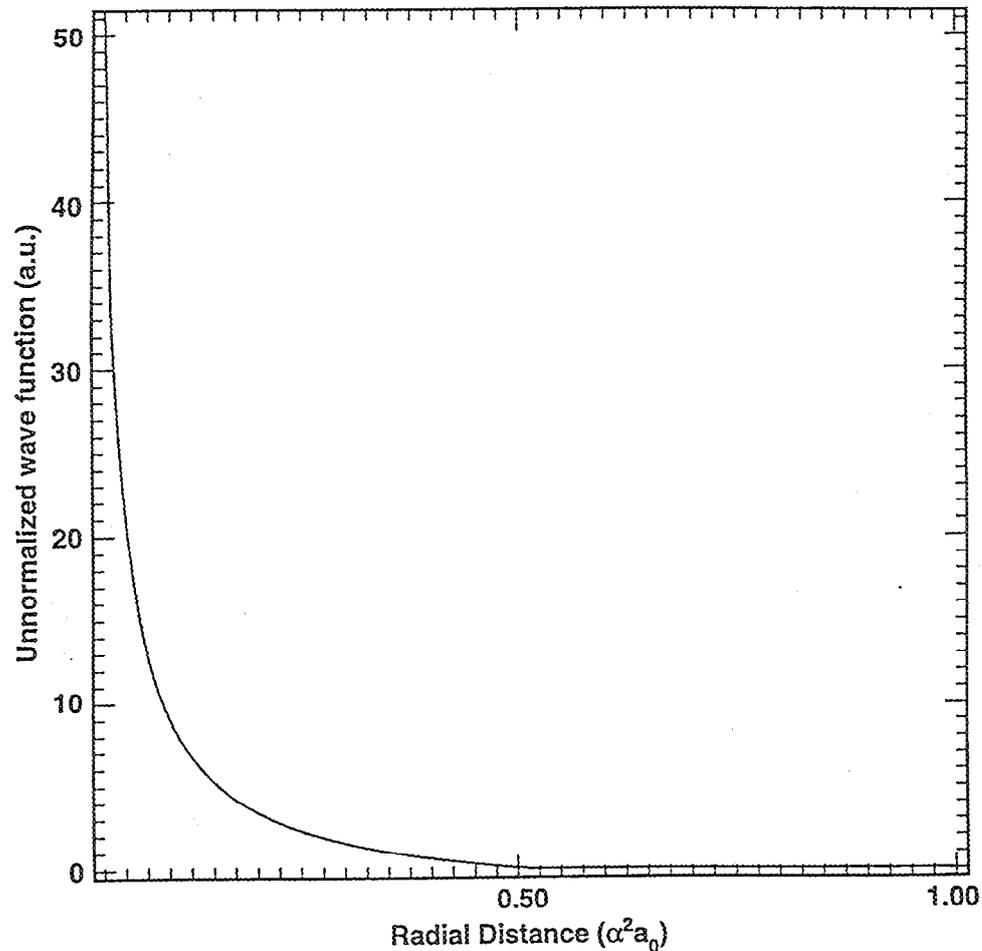


Figure 4. Example of Dirac-like ansatz used to fill up the Lorentz relativistic wave equation (LRWE) spectral subregion in the regime  $-\infty < E < -mc^2$ . The plot shows the wave function versus radial distance for a cut off at the origin of  $0.0195 \alpha^2 a_0$  (where  $\alpha$  is the fine structure constant and  $a_0$  the bohr radius) and boundary condition that the wave function vanish at  $\alpha^2 a_0/2$ . The LRWE is satisfied for an energy of  $-0.804022490267 mc^2$ . The number of significant figures shows the sensitivity to the boundary condition.