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Critical coupling constants for relativistic wave equations and vacuum breakdown in quantum electrodynamics

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We study the strong-coupling limit of some relativistic wave equations describing bound states of oppositely charged fermions or bosons 1 and 2, of arbitrary mass. Using both numerical and analytic momentum-space methods we find the value $\gamma_{\rm max}$ of $\gamma=-e_1e_2/4\pi$ for which the lowest-lying bound state disappears from the spectrum, as well as the smaller value $\gamma_{\rm dec}$ for which 2 becomes unstable to the decay into the composite (1,2) system and the antiparticle $\bar{1}$. We also consider the limit $m_2\to\infty$ and discuss the connection of our results with the so-called breakdown of the vacuum in quantum electrodynamics for a sufficiently strong external field.

I. INTRODUCTION

The study of relativistic wave equations describing bound states of interacting particles is an old but still active topic. An aspect of such equations which has received renewed attention in recent years is their behavior for large values of the associated coupling constant. In some cases there is a maximum strength beyond which one or more bound states disappear from the spectrum and the physical interpretation of the equation becomes obscure. The most familiar example is provided by the Dirac equation for a one-electron atom,

$$H_{D;{\rm ext}}\psi=(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta m+V_{\rm ext})\psi=E_D\psi\ . \qquad (1.1)$$

For a point nucleus of charge Ze, $V_{\rm ext}=-\alpha Z/r$ and the $1s$ state has energy

$$E_D(1s)=m(1-\gamma^2)^{1/2}\ ,\quad \gamma\equiv\alpha Z\ .$$

$E_D(1s)$ vanishes for $\gamma=1$ and becomes imaginary for $\gamma>1$, while the higher-lying $j=\frac{1}{2}$ state energies become complex. For general values of j the critical value of γ is $j+\frac{1}{2}$. If the point Coulomb potential is spread out by giving the source a size appropriate for a physical nucleus of charge Ze, this situation changes: $E_D(1s)$ now vanishes for a somewhat larger value, $\gamma\simeq1.10$, corresponding to $Z\simeq150$, but for still larger γ becomes negative rather than imaginary. $E_D(1s)$ reaches the value $-m$, for a critical value $\gamma\simeq1.24$ ($Z\simeq170$). These matters and related problems such as the two-center Dirac equation have been the object of intense study over the past decade in connection with the prediction of anomalous pair production in heavy-ion collisions and the associated "vacuum breakdown" in the presence of super-heavy nuclei.[1]

It is natural to ask whether these features of the c-number external-field Dirac equation are in any way associated with the fact that the spectrum of $H_{D;{\rm ext}}$ is not bounded below. One may also wonder to what extent the conclusions drawn from the external-field Dirac equation remain unchanged when the finite mass of the source is taken into account. In this case one should also consider the effect of including transverse photon exchange between the source and the electron. One purpose of this paper is to address these questions.

Our task is facilitated by a recent numerical study of a two-body relativistic wave equation which provides an approximate description of bound states of two fermions of arbitrary masses, m_1 and m_2, while reducing in the limit $m_2\to\infty$ to an equation simply related to the external-field Dirac equation.[2] This equation has the form, in the c.m. system,

$$[h_D(1)+h_D(2)+\Lambda_{++}V\Lambda_{++}]\psi=E\psi\ , \qquad (1.2)$$

where

$$h_D(i)=\boldsymbol{\alpha}_i\cdot\mathbf{p}_i+\beta_i m_i \qquad (1.2a)$$

is the free one-particle Dirac Hamiltonian, with $\mathbf{p}_1=-\mathbf{p}_2=\mathbf{p}$ and

$$\Lambda_{++}=\Lambda_+(1)\Lambda_+(2) \qquad (1.2b)$$

is the product of the Casimir positive-energy projection operators

$$\Lambda_+(i)=[E_i+h_D(i)]/2E_i \qquad (1.2c)$$

with $E_i=(m_i^2+\mathbf{p}_i^2)^{1/2}$. The wave function ψ satisfies the constraints $\Lambda_+(i)\psi=\psi$ so that the spectrum of (1.2) is bounded below, unlike that of (1.1) or of the related Dirac-Breit equation, obtained from (1.2) by omitting the projection operators.

In Ref. 2 the eigenvalue E associated with the $1s$ ground state of (1.2) was found for two choices of the potential V, a Coulomb potential V_C and the sum V_C+V_B of V_C and a Breit potential V_B:

$$V_C=-\gamma/r\ ,\quad V_B=(\gamma/2r)(\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2+\boldsymbol{\alpha}_1\cdot\hat{\mathbf{r}}\,\boldsymbol{\alpha}_2\cdot\hat{\mathbf{r}})\ , \qquad (1.3)$$

and the dependence of E on the coupling strength

$$\gamma = | e_1 e_2 | /4\pi \tag{1.4}$$

was studied for small to intermediate values of γ. In the present paper we extend this to $\gamma \sim 1$ and study the critical values of γ from both a numerical and analytic point of view. We also report similar results for analogous equations involving spinless particles and comment on one aspect of some recent work on two-body bound-state equations for such particles.[3,4] The extent to which the use of such equations as (1.2) or the closely related Bethe-Salpeter equation represents an adequate approximation to the physical situation involved in the strong-coupling regime is not known. We regard (1.2) with V a one-photon-exchange potential as a reasonable starting point for the exploration of the effects of recoil in this regime at the present state of knowledge and our study as a first step in this direction.

We now outline the contents of the following sections. In Sec. II we first reconsider the question of critical constants for the Dirac equation, in momentum space rather than coordinate space, as a test of the techniques we shall employ. We then study the same problem for the no-pair analog of the Dirac equation,

$$h_+(1)\psi = [h_D(1) + \Lambda_+(1) V \Lambda_+(1)]\psi = E_+ \psi \ , \tag{1.5}$$

which is the $m_2 = \infty$ limit of (1.2). Our study of critical coupling constants for the no-pair two-body equation (1.2) is described in Sec. III; we emphasize that in the case of the two-body problem, unlike the external-field problem, one must be careful to distinguish between several different kinds of "critical values" for coupling strengths, including the value γ_{dec} for which E equals $m_2 - m_1$ and the value $\gamma_{\max}$ for which the expectation value of the potential V diverges. In Sec. IV our study is extended to some two-body equations for spinless particles. A summary of our results and a concluding discussion are given in Sec. V. The mathematical analysis needed for the determination of the critical coupling constants is described in Appendix A. Some mathematical aspects of the Dirac equation, which relate to the question of the self-adjointness of $H_{D;\text{ext}}$ for large γ, are discussed in Appendix B.

II. EXTERNAL-FIELD EQUATIONS: SPIN $\frac{1}{2}$

A. Dirac equation

As mentioned above, the value $\gamma = 1$ is critical for the Dirac equation with a Coulomb potential, since $E_D(1s)$ becomes complex for $\gamma > 1$. For our later purpose we note the less well-known fact that the value $\gamma_* = \sqrt{3}/2 \simeq 0.87$ is also significant. For $j = \frac{1}{2}$ and $\gamma < \gamma_*$ there is another solution ψ', with the same energy as the usual one, which does not belong to the Hilbert space and, *a fortiori,* is not in the domain of $H_{D;\text{ext}}$, because it is too singular at the origin to be square integrable. However, for $\gamma > \gamma_*$ the function ψ' also becomes square integrable and is excluded from the domain only by the requirement that the expectation value of the potential V be finite on the domain in Hilbert space on which the Hamiltonian $H_{D;\text{ext}}$ is defined. This restriction then leads to a domain on which $H_{D;\text{ext}}$ is self-adjoint.[5]

These matters have been discussed in the literature from the viewpoint of the familiar coordinate-space formulation of the Dirac equation. Let us see how they appear in momentum space. In Appendix A we outline a derivation of the connection between the value of γ and the asymptotic behavior of the solutions of a variety of relativistic wave equations, considered in $\mathbf{p}$ space, for large $|\mathbf{p}|$. As a check for the cases to be treated later, where analytic solutions are not available, we have applied this technique to (1.1) written in $\mathbf{p}$ space, viz.,

$$(\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m)\tilde{\psi}(\mathbf{p}) - \frac{\gamma}{2\pi^2}\int \frac{d\mathbf{p}'}{(\mathbf{p}-\mathbf{p}')^2}\tilde{\psi}(\mathbf{p}') = E_D \tilde{\psi}(\mathbf{p}) \ . \tag{2.1}$$

With $\tilde{\psi}(\mathbf{p})$ assumed to vary as $p^{-2-\nu}$ for $|\mathbf{p}| \to \infty$, one finds that the $j = \frac{1}{2}$ solutions must satisfy [see (A17)]

$$\gamma^2 = 1 - \nu^2 \ . \tag{2.2}$$

One readily verifies that $\langle V_C \rangle$ diverges for $\text{Re}\nu \le 0$, so that $\gamma_{\max} = 1$ as expected. As a test of our methods we have extended the numerical solution of (2.1), carried out in Ref. 2 for $\gamma \le 0.9$, to larger values of γ and, using the onset of numerical instability and the growth of $\langle V_C \rangle$ as criteria, found $\gamma_{\max}^{\text{num}} = 0.99 \pm 0.01$. We have also solved (2.1) with $(\mathbf{q})^{-2} = (\mathbf{p}-\mathbf{p}')^{-2}$ replaced by $(\mathbf{q})^{-2} - (\mathbf{q}^2 + \mu^2)^{-1}$, corresponding to a smoothed-out potential

$$-\gamma(1 - e^{-r/R})/r \ , \tag{2.3}$$

where $R = \mu^{-1}$ is the nuclear radius. We have verified that the $1s$ state wave function continues to be associated with a real eigenvalue for $\gamma > 1$, which reaches the value $-m$ for sufficiently large γ. This is in qualitative agreement with the results obtained in $\mathbf{r}$ space for more realistic potentials.[1]

B. No-pair external field equation

After these preliminaries we are ready to consider (1.5), the no-pair analog of (2.1). In $\mathbf{p}$ space Eq. (1.5) takes the form

$$(\mathbf{p}^2 + m^2)^{1/2}\tilde{\psi}(\mathbf{p}) - \frac{\gamma}{2\pi^2}\Lambda_+(\mathbf{p})\int \frac{d\mathbf{p}'}{(\mathbf{p}-\mathbf{p}')^2}\Lambda_+(\mathbf{p}')\tilde{\psi}(\mathbf{p}') = E_+ \tilde{\psi}(\mathbf{p}) \ , \tag{2.4}$$

since ψ is subject to the constraint $\Lambda_+\psi = \psi$. We have again extended the numerical calculations of Ref. 2 to values of γ above 0.9. Using the same criteria as in the pure Dirac case we have found that the maximum value of γ for the $1s$ state is not much larger than 0.9,

$$0.90 < \gamma_{\max} < 0.93 \ . \tag{2.5}$$

Within numerical uncertainties, $\gamma_{\max}$ is also the value γ_0 for which E_+ vanishes:

$$\gamma_0 \approx \gamma_{\max} \ . \tag{2.6}$$

As shown in Appendix A, the relation between the exponent ν in the asymptotic behavior $p^{-2-\nu}$ of the $j=\frac{1}{2}$ bound states, and the coupling strength γ is now given by [see (A9), (A10), and (A19)]

$$\gamma(\nu)=2\Big/\left[\nu^{-1}\tan\frac{\pi\nu}{2}+\frac{\nu}{1-\nu^2}\cot\frac{\pi\nu}{2}\right] . \tag{2.7}$$

The variation of γ with ν in the interval $(-1,1)$ is shown in Fig. 1. The maximal value of γ occurs, as in the Dirac case, for $\nu=0$,

$$\gamma_{\max}=2\Big/\left[\frac{\pi}{2}+\frac{2}{\pi}\right]\simeq 0.906 . \tag{2.8}$$

Thus the result (2.5) is consistent with theoretical expectations.

For a given value of $\gamma<\gamma_{\max}$ there are, as for the Dirac equation, two solutions of the same energy, $\tilde{\psi}(\mathbf{p})$ and $\tilde{\psi}'(\mathbf{p})$ corresponding to positive and negative values of ν, respectively, with only $\tilde{\psi}(\mathbf{p})$ normalizable for all γ. The value γ_* above which $\tilde{\psi}'(\mathbf{p})$ becomes normalizable is given by putting $\nu=-\frac{1}{2}$ in (2.7):

$$\gamma_*=\gamma(-\tfrac{1}{2})=\tfrac{3}{4} . \tag{2.9}$$

We see from these results that the absence of a lower bound for the spectrum of the Dirac Hamiltonian with a point source is *not* related to the existence of a maximal value for γ since the spectrum of h_+, defined by the left-hand side of (2.4), *is* bounded below. The fact that both γ's are smaller than their counterparts for $H_{D;\text{ext}}$ [$\gamma_{\max}=1$ and $\gamma_*=\sqrt{3}/2$] is a consequence of the circumstance that the effects of virtual pair creation, omitted in (2.4) but included in (2.1), are equivalent to a repulsive interaction of fermion 1 with the infinitely massive core 2.

III. TWO-BODY EQUATIONS: SPIN $\frac{1}{2}$

A. Definition of "critical" coupling constants

Let $E=E(\gamma;m_1,m_2)$ denote an eigenvalue of any relativistic two-body equation, which may be interpreted as the mass of a bound two-body system (1,2). The variable γ denotes a parameter describing the strength of the binding interaction, with $\gamma \gtrsim 0$ in the weak coupling limit, where $E \lesssim m_1+m_2$. We define several critical values of γ as follows. With $m_2 \geq m_1$, it may be possible to increase γ to a value γ_{dec} above which particle $\underline{2}$ becomes unstable to the decay

$$2\to(1,2)+\bar{1} , \tag{3.1}$$

where the bar denotes an antiparticle. This value is determined by

$$E(\gamma_{\text{dec}};m_1,m_2)=m_2-m_1 . \tag{3.2}$$

It may be also possible to increase γ to a value beyond which the equation loses its normal physical interpretation. We will refer to any such value as a $\gamma_{\max}$. For example, if the equation is of Hamiltonian form

$$H\psi=(K_1+K_2+\gamma U)\psi=E\psi , \tag{3.3}$$

where K_i is the free Hamiltonian for particle $\underline{i}$, then $\gamma_{\max}$ may be defined as that value above which H is no longer self-adjoint on a dense domain. Guided by experience with the Dirac equation, we may alternatively use a more practical definition of $\gamma_{\max}$ as a value of γ with the property that the expectation value function

$$X(\gamma)=\langle\psi\,|\,U\,|\,\psi\rangle \tag{3.4}$$

is well-defined for all $\gamma<\gamma_{\max}$, but such that $X(\gamma)$ diverges as $\gamma\to\gamma_{\max}$ from below for at least one (normalizable) eigenfunction of H,

$$\gamma_{\max}\text{:}\;\; X(\gamma)\to\infty \;\;\text{for } \gamma\to\gamma_{\max} . \tag{3.5}$$

We will assume as a working hypothesis that these two definitions are equivalent in the cases of interest to us. In addition, one may wish to consider a value γ_0 for which E vanishes and a value γ_* analogous to that considered in Sec. II for the Dirac equation, but such values, if they exist, play at best a secondary role.

To deal with the case $m_2 \gg m_1$, it is useful to define an effective one-body energy $E(\gamma;m_1)$ via

$$E(\gamma;m_1)=\lim_{m_2\to\infty}[E(\gamma;m_1,m_2)-m_2] . \tag{3.6}$$

If $E(\gamma;m_1,m_2)$ is defined by an equation of the form (3.3) and the limits involved exist, then $E(\gamma;m_1)$ is determined by

$$(K_1+\gamma U')\psi'=E(\gamma;m_1)\psi' \tag{3.7}$$

where U' and ψ' are the $m_2=\infty$ limits of U and ψ, respectively. Correspondingly, in analogy with (3.2) we define a γ'_{dec} for the associated one-body problem by

$$E(\gamma'_{\text{dec}};m_1)=-m_1 \tag{3.8}$$

with

$$\gamma'_{\text{dec}}=\lim_{m_2\to\infty}\gamma_{\text{dec}} . \tag{3.9}$$

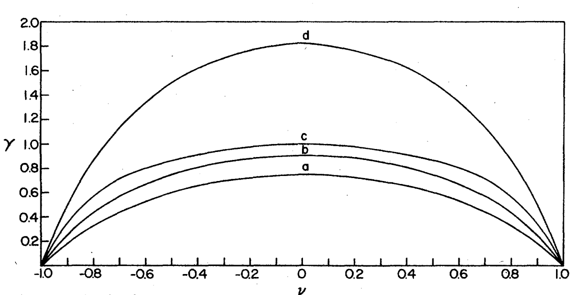

FIG. 1. Relation between the coupling strength γ entering the bound-state equations and the exponent ν describing the large-p behavior, $p^{-2-\nu}$, of the corresponding ground-state wave functions. Curves (a) two-body no-pair equation (1.2), with $V=V_C+V_B$, (b) no-pair external-field equation (2.4), (c) Dirac equation (2.1), (d) two-body no-pair equation (1.2), with $V=V_C$.

B. Results

In Ref. 2 the dependence of the $1\,^1S_0$-state eigenvalue E of (1.2) on γ was studied, for the case $m_1=m_2$, in the range $0<\gamma<0.6$ and for two choices of V:

$$V=V_C \qquad (3.10)$$

and

$$V=V_C+V_B\ , \qquad (3.11)$$

where V_C and V_B are defined by (1.3). The results of the extension of this analysis to larger values of γ and to different values of the mass ratio $\eta=m_2/m_1$ are shown in Figs. 2 and 3.

1. $V=V_C$

We see from Fig. 2 that when η is unity

$$\gamma_{\max}^{\text{num}}\simeq 1.86\ . \qquad (3.12)$$

The asymptotic analysis of Appendix A yields [see (A21)]

$$\gamma(\nu)=4\Big/\left[\nu^{-1}\tan\frac{\pi\nu}{2}+\frac{\nu}{1-\nu^2}\cot\frac{\pi\nu}{2}\right] \qquad (3.13)$$

from which it follows that

$$\gamma_{\max}=\gamma(0)=4\Big/\left[\frac{\pi}{2}+\frac{2}{\pi}\right]\simeq 1.81\ , \qquad (3.14)$$

with which (3.12) is in agreement, within a few percent.

The analysis of Appendix A shows that (3.13) and hence (3.14) holds for any value of $\eta<\infty$, not just $\eta=1$. The curves shown in Fig. 2 are indeed consistent with the independence of $\gamma_{\max}$ on the mass ratio η. However, for $\eta=\infty$, $\gamma(\nu)$ is given by (2.7), which is just one-half the

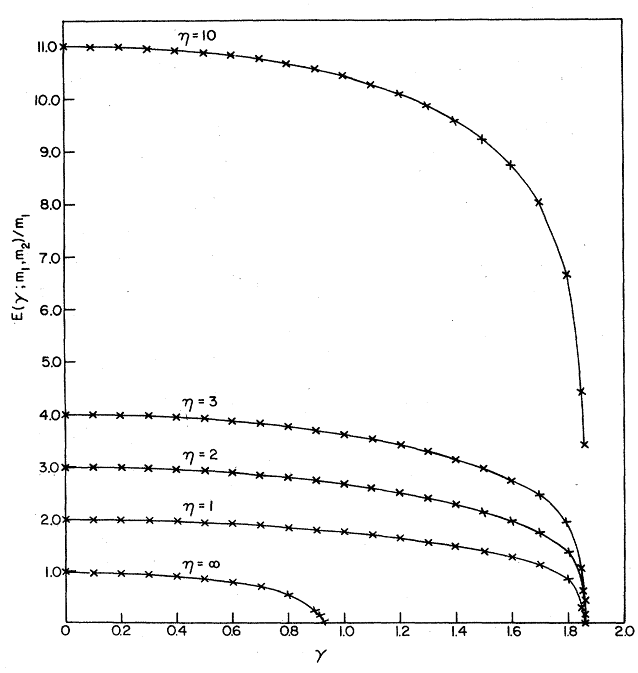

FIG. 2. Mass of the lowest-lying bound state, in units of m_1, vs coupling strength γ for the two-body no-pair equation (1.2), with $V=V_C$; the quantity η denotes the mass ratio m_2/m_1. The curve labeled $\eta=\infty$ is a plot of the ratio $E(\gamma;m_1)/m_1$ whose numerator is defined by Eq. (3.6) of the text.

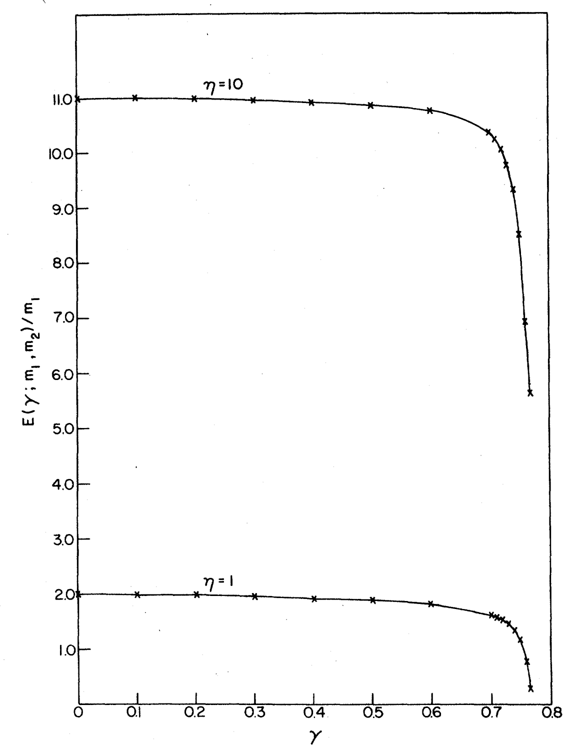

FIG. 3. Mass of the lowest-lying bound state, in units of m_1, vs coupling strength γ for the two-body no-pair equation (1.2), with $V=V_C+V_B$.

value (3.14). *A fortiori,* the factor $\frac{1}{2}$ also relates the two values of $\gamma_{\max}$. *Thus the double limit,* $p\to\infty$, $\eta\to\infty$, *depends on the order in which it is taken.*

Let us now turn to the quantity γ_{dec}, defined by Eq. (3.2), i.e., the value of γ above which 2 becomes unstable against the decay process (3.1). For $\eta=1$, Eq. (3.2) shows that γ_{dec} coincides with the value γ_0 for which $E=0$. From Fig. 2 we see that $\gamma_0\simeq 1.86$ so that also

$$\gamma_{\text{dec}}^{\text{num}}(\eta=1)\simeq 1.86 \qquad (3.15)$$

which is equal to $\gamma_{\max}$, within numerical uncertainty. We also see from Fig. 2 that $\gamma_{\text{dec}}(\eta)$ decreases as η increases, having approximate numerical values of 1.86, 1.80, and 1.60 for $\eta=2$, 3, and 10, respectively. We have also verified that for $\eta=100$, $\gamma_{\text{dec}}\simeq 1.25$ (not shown in Fig. 2). Thus we see that $\gamma_{\text{dec}}(\eta)$ decreases very slowly as η increases, presumably always remaining larger than $\gamma_{\max}$ for the $m_2=\infty$ limit, given by Eq. (2.8). In a further study it would be interesting to investigate the behavior of $\gamma_{\text{dec}}(\eta)$ for very large η and to compare the limiting value γ'_{dec} defined by (3.9) with the value of $\gamma_{\max}$ when $m_2=\infty$.

2. $V=V_C+V_B$

In Fig. 3 we show the results analogous to those of Fig. 2 for this choice of V. As already noted in Ref. 2 for the equal-mass case, inclusion of the Breit operator lowers the energy. Thus one expects that $\gamma_{\max}$ is reduced relative to its value for a pure Coulomb potential for any value of the mass ratio η. From Fig. 3 we see that when η is unity,

γ_{max} is not much larger than 0.74,

$$0.74 < \gamma_{max}^{num} < 0.77 , \quad (3.16)$$

and so is indeed smaller than the pure Coulomb value, given by (3.12). Equation (3.16) is consistent with the result obtained from the asymptotic analysis of Appendix A, which gives [Eq. (A22)]

$$\gamma(\nu)=4\Big/\left[3\nu^{-1}\tan\frac{\pi\nu}{2}+\frac{\nu}{1-\nu^2}\cot\frac{\pi\nu}{2}\right] \quad (3.17)$$

and therefore

$$\gamma_{max}=\gamma(0)=4/(3\pi/2+2/\pi)\simeq 0.748 . \quad (3.18)$$

As in the pure Coulomb case, the asymptotic analysis leading to (3.18) holds for $1 \le \eta < \infty$. But here too $\gamma(\nu)$ is given by (2.7) for $\eta=\infty$ and again we see that the double limit $p\to\infty, \eta\to\infty$ depends on the order in which it is taken.

The quantity γ_{dec} for the case when $V=V_C+V_B$ appears to remain close to the value γ_{max}, as can be inferred from Fig. 3. There we see that $\gamma_{dec}^{num}(\eta)\approx 0.75$ even for $\eta=10$. We have found that for $\eta=100$, $\gamma_{dec}^{num}(\eta)\simeq 0.72$, so that $\gamma_{dec}(\eta)$ is again a very slowly varying function of η.

IV. TWO-BOSON BOUND STATES

It is of some interest to see what the results analogous to those of Sec. III are for the case of two spin-0 particles. Instead of (1.2) we now have

$$[E_1(\mathbf{p}_1)+E_2(\mathbf{p}_2)+V_C]\phi=E\phi , \quad (4.1)$$

where $\mathbf{p}_1=-\mathbf{p}_2=\mathbf{p}$ as before and we restrict our attention to a pure Coulomb interaction.

A. External-field limit

With $E=E(\gamma;m_1)$ defined as in (3.6), the $m_2=\infty$ limit of (4.1) is

$$[E_1(\mathbf{p}_1)+V_C]\phi=E\phi . \quad (4.2)$$

Figure 4 shows the dependence of E on γ, obtained by numerical solution of (4.2), from which we see that

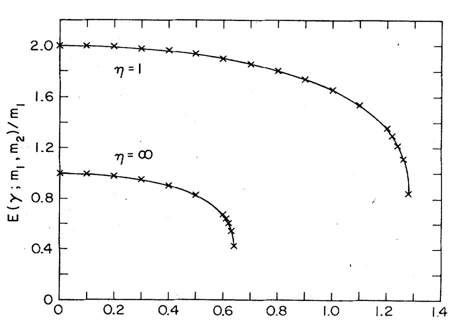

FIG. 4. Mass of the lowest-lying bound state, in units of m_1, vs coupling strength γ for the spin-0 two-body equations (4.1) ($\eta=1$) and (4.2) ($\eta=\infty$). The lower curve is a plot of the eigenvalue of the one-body equation (4.2), in units of m_1.

$$\gamma_{max}^{num}\simeq 0.65 . \quad (4.3)$$

From Eq. (A16) of Appendix A we have

$$\gamma(\nu)=\pi/F_0(\nu)=\nu\Big/\tan\frac{\pi\nu}{2} \quad (4.4a)$$

so that

$$\gamma_{max}=2/\pi\simeq 0.637 . \quad (4.4b)$$

Thus (4.3) is consistent with expectations. Equation (4.4b) has also been obtained by Castorina *et al.*,[4] who used **r**-space methods to study Eq. (4.1) and, much earlier, by Herbst,[6] who has developed the spectral theory of (4.2) on a rigorous basis.

B. Genuine two-body case

We only consider $m_1=m_2=m$. The results of calculation are shown in Fig. 4, from which one sees that

$$\gamma_{max}^{num}\simeq 1.28 . \quad (4.5)$$

The asymptotic analysis of Appendix A or more simply a rescaling of (4.2) shows that γ_{max} is just twice the value found in the external-field limit:

$$\gamma_{max}=4/\pi\simeq 1.274 , \quad (4.6)$$

consistent with (4.5). Although we have not calculated $E(\gamma;m_1,m_2)$ for $\eta\neq 1$, Eq. (A16) shows that γ_{max} is independent of η and hence given by (4.6) for all $\eta<\infty$.

The result (4.6) is in conflict with some recent work of Durand and Durand[3] who have made an extensive study of Eq. (4.1) in the equal mass case and claim to have found a closed formula for the lowest eigenvalue of (4.1), viz.,

$$E=2m\Big/\left[1+\frac{\gamma^2}{4}\right]^{1/2} . \quad (4.7)$$

If (4.7) were valid one would infer that

$$\gamma_{max}=\infty , \quad (4.8)$$

so that there is no maximum value of γ, in contradiction with (4.5) or (4.6). However, (4.7) also disagrees with perturbation theory. The leading correction to the nonrelativistic energy $W_0=-\gamma^2/4m$ is given by

$$\delta^{(4)}E=-\frac{1}{4m^3}\langle\phi_0|p^4|\phi_0\rangle=-\frac{1}{4m^3}\langle p^2\phi_0|p^2\phi_0\rangle , \quad (4.9)$$

where ϕ_0 is the nonrelativistic wave function. It is clear from the second form of (4.9) that $\delta^{(4)}E$, which arises from the difference between the relativistic and nonrelativistic form of the operator for the kinetic energy, is negative whereas the term of $O(\gamma^4)$ obtained from expansion of (4.7), viz.,

$$+\tfrac{3}{64}\gamma^4 m , \quad (4.10)$$

is positive. Evaluation of (4.9) yields

$$\delta^{(4)}E=-\tfrac{5}{64}\gamma^4 m . \quad (4.11)$$

[In Ref. 3 it is stated that perturbation theory gives the result (4.10), in agreement with Eq. (4.7); one can get the result (4.10) if one uses the first form of (4.9) in coordinate space, but only if one omits a δ-function term arising in the evaluation of $\nabla^2(\nabla^2\phi)$.[7]

As a further check on the numerical accuracy of the curve shown in Fig. 4, at least for small γ, we have used it to find the limit,

$$\lim_{\gamma\to 0}\left[E-\frac{\gamma^2}{4}m\right]\Big/\gamma^4 \simeq -0.0781 \ . \qquad (4.12)$$

This is in very good agreement with (4.11) since $\frac{5}{64}\simeq 0.078\,125$.

V. SUMMARY AND DISCUSSION

We have studied the question of critical coupling constants for a number of relativistic wave equations in this paper. With regard to one-body equations, in Sec. II we first used the **p**-space approach described in Appendix A to recover the familiar result that $\gamma_{\max}=1$ for the Dirac-Coulomb equation, from the requirement that $\langle V_C \rangle$ be finite. We then demonstrated that the absence of a lower bound for the spectrum of the Dirac-Coulomb Hamiltonian $H_{D;\text{ext}}$ is not related to the existence of a $\gamma_{\max}$ by showing that the no-pair equation (2.4), for which the spectrum is bounded below, also has a $\gamma_{\max}$. It was seen that for this equation, as for the Dirac equation, $\gamma_{\max}$ coincides with the value γ_0 for which the lowest-lying bound-state energy vanishes. In both cases the values of $\gamma_{\max}$ found numerically were in good agreement with the theoretically expected values. We also obtained in each case the value γ_* above which the condition that $\langle V_C \rangle$ be finite serves to ensure that the Hamiltonians involved are self-adjoint on their domains.

In Sec. III we turned to the two-body problem. We saw that one should distinguish in this case among a variety of critical values of the coupling constant γ: the value $\gamma_{\max}$ for which the expectation value of the interaction operator first diverges, the value γ_{dec} above which the heavier constituent 2 becomes unstable to the decay $2\to(1,2)+\bar{1}$ and the value γ_0, if any, for which the mass of the bound state (1,2) vanishes. When $V=V_C$, a pure Coulomb potential, we found on the one hand that for $m_2\geq m_1>0$, $\gamma_{\max}=\gamma_{\max}(\eta)$ is given by (3.14), for any value of the mass ratio $\eta\equiv m_2/m_1<\infty$. This is however twice the value found for $\eta=\infty$ from the solution of the one-body equation (2.4), obtained by taking the limit $m_2\to\infty$ in the two-body equation. Thus $\gamma_{\max}(\eta)$ is a discontinuous function of $\zeta=1/\eta$ in the neighborhood of $\zeta=0$. On the other hand, study of $\gamma_{\text{dec}}(\eta)$ showed that the initial value $\gamma_{\text{dec}}(1)=\gamma_{\max}(1)$ decreases with increasing η. However, this decrease is very slow, with γ_{dec} decreasing by only a factor of $\frac{2}{3}$ as η increases from 1 to 100.

These results change considerably when the effect of transverse photon exchange is approximately included in V by adding the Breit operator to V_C. Again $\gamma_{\max}(\eta)$ is independent of η for $\gamma<\infty$, but its value, given by Eq. (3.19), is smaller than in the pure Coulomb case by more than a factor of 2. This can be understood qualitatively from the observation that the inclusion of transverse photon exchange makes the effective interaction in the $^1S_0$ state more attractive. A simple way to see this is to consider the Möller form of the total one-photon-exchange potential, viz., $V_M=(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)V_C$. Since $\boldsymbol{\alpha}_i\sim\mathbf{p}_i/E_i$ and $\mathbf{p}_1=-\mathbf{p}_2=\mathbf{p}$ in the c.m. system, at large momenta V_C is enhanced by a factor of order $1+\mathbf{p}^2/E^2\sim 2$. [A more careful analysis, similar to that used in Appendix A, reveals that Eq. (1.2) with $V=V_M$ leads to $\gamma_{\max}=2/\pi$ so that V_C is effectively enhanced by a factor of 3.] For the Breit form the calculation is more complicated (see Appendix A) but the net effect is similar, with V_C enhanced by a factor of 2.4. Although $\gamma_{\text{dec}}(\eta)$ certainly exists for some range of η, the behavior of the quantity $\gamma_{\text{dec}}(\eta)$ is somewhat problematic for $V=V_C+V_B$. From Fig. 3, we see that when $\eta=10$, $\gamma_{\text{dec}}\sim 0.74$ to 0.75, very close to the value $\gamma_{\max}=0.748$, but our numerical accuracy is really not sufficiently high for us to be certain that γ_{dec} exists for this value of η. For $\eta=100$, we have found a numerical value $\gamma_{\text{dec}}\sim 0.72$ which may represent a real solution of the equation defining γ_{dec}. Whatever the case, $\gamma_{\text{dec}}(\eta)$ is again a very slowly varying function of η in the region where it exists.

In Sec. IV we studied the spin-0 analog of the one- and two-body spin-$\frac{1}{2}$ equations, considered in Secs. II and III, for the case of a pure Coulomb interaction. We found the values of $\gamma_{\max}$ in both cases, and the variation with γ of the ground-state energy $E(\gamma;m_1)$ of the one-body equation (4.2), exhibited in Fig. 4. From Fig. 4 and the underlying numerical work we have no evidence that $E(\gamma;m_1)\to 0$ as $\gamma\to\gamma_{\max}$. If anything, the indications are that it does not. If so, this is in striking contrast to both the Dirac equation and the no-pair equation (1.5). It would be interesting to eludicate further this apparent distinction between the spin-0 and spin-$\frac{1}{2}$ case by use of analytical rather than numerical methods. Our numerical results for (4.2) are consistent with the lower bound given by Herbst,[6]

$$E(\gamma;m)\geq[1-(\gamma/\gamma_{\max})^2]^{1/2}m \ ,$$

where $\gamma_{\max}=2/\pi$. As a by-product we saw that the analysis of Eq. (4.1) given in Ref. 3 requires modification, and that an exact formula for the lowest eigenvalue of (4.1) or (4.2) is still not on the market.

We note in passing that Herbst comments on the relative neglect of the study of the one-body square-root equation, augmented by an interaction with a magnetic field with vector potential $\mathbf{A}(\mathbf{x})$, viz.,

$$\{[(\mathbf{p}-e\mathbf{A})^2+m^2]^{1/2}-eA_0(\mathbf{x})\}\phi(\mathbf{x})=E\phi(\mathbf{x}) \ , \qquad (5.1)$$

compared to the Klein-Gordon (KG) equation. This is so despite the fact that in contrast to the KG equation, (5.1) is of Hamiltonian form and, in the pure Coulomb case, allows a larger range of values of Z ($\gamma_{\max}=\frac{1}{2}$ for the KG equation which is less than $2/\pi$). Herbst ventures the opinion that the main reason for this is that, unlike the KG equation, (5.1) is not explicitly solvable even for the pure Coulomb case. While this may very well be correct, from a sociological point of view, we take the occasion to emphasize that, as shown long ago, Eq. (5.1) with E replaced by $i\partial/\partial t$ and $\phi(\mathbf{x})\to\phi(x)=\phi(\mathbf{x},t)$ is not invariant under Lorentz transformations, with $\phi(x)$ a world scalar, unlike the time-dependent KG equation.[8] Thus, the comparative neglect of (5.1) may to some extent be regarded as benign. Indeed, the noninvariance of the square-root KG equation, when the minimal principle is used to generate interactions with an external electromagnetic field, is cited by Dirac, when he presents the reasoning which leads to the relativistic wave equation for an electron.[9]

In conclusion let us comment on some other features of our results which merit further study.

We have already mentioned that in the two-body pure Coulomb case the function $\gamma_{\max}(\eta)$ is, on the one hand, independent of the mass ratio $\eta=m_2/m_1$ for $0<\eta<\infty$. On the other hand, its constant value (~ 1.81) is not equal to the value of $\gamma_{\max}(\infty)$ $[m_2=\infty, m_1>0]$, i.e., to the value appropriate for the external field problem, being in fact twice as large. We have also seen that the inclusion of transverse photons can have a significant effect on $\gamma_{\max}$. Now quantities analogous to $\gamma_{\max}(\infty)$ have been used in predicting the onset of "vacuum breakdown" in the collision of heavy ions or subsequent to the production of superheavy nuclei, as manifested by the anomalous production of positrons. Thus, there appears at first sight to be some danger that the neglect of recoil as well as the neglect of transverse photon exchange might lead to a substantial change in the critical values of Z needed for such experiments. However, one must remember that the point charge cases we have studied in this paper are an idealization of the actual physical situations which involve nuclei with distributed charge and that the replacement of point charges by distributed charges can have, as it does in the external-field Dirac equation, a drastic effect on the bound-state spectrum for large Z values and hence on the values of critical coupling constants. Thus, it would be premature to draw any conclusions from our results with regard to the validity of the extant theoretical analyses of the experiments in question. Nevertheless, the discontinuity between the $m_2<\infty$ and $m_2=\infty$ values for $\gamma_{\max}$ suggests that one's understanding of the physical significance of this quantity is incomplete. It may be that further study of the behavior of $\gamma_{\rm dec}(\eta)$ for large η, together with the inclusion of distributed charge and virtual pair effects will ameliorate this. In view of the interest attached to these topics such an extension of our analysis would appear to be a worthwhile project.

As a final remark, let us see how the anomalous production process in, say, U-U collisions would be described in terms of the concept of the "decay coupling strength" $\gamma_{\rm dec}$ introduced in Sec. III A. There $\gamma_{\rm dec}$ was defined as a value, if any, such that

$$E(\gamma;m_1,m_2)-m_2\le -m_1 \quad (\gamma\ge\gamma_{\rm dec})$$

where E is the mass of the lowest (1,2) bound state. With $m_1=m_e$ and m_2 identified as the mass M^* of an excited U-U complex X^* formed during the collision, we can envisage the process

$$\mathrm{U}+\mathrm{U}\to X^* .$$

This can be followed by the decay

$$X^*\to(X^*,e^-)+e^+$$

provided that $\gamma=\alpha Z^*$ exceeds the value $\gamma_{\rm dec}$ determined by the equation

$$E(\gamma_{\rm dec};m_e,M^*)-M^*=-m_e .$$

Note that in this way of looking at the process we have not needed to make any explicit reference to the vacuum state or to the concept of "vacuum breakdown."

Note added in proof. The authors of Ref. 3 have informed us that they agree with our criticism of Eq. (4.7).

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APPENDIX A: COUPLING CONSTANT BOUNDS FROM p-SPACE EQUATIONS

1. Preliminaries

The action of the Coulomb potential $V_C(r)=-\gamma/r$ on a function which has the form, in $\mathbf{p}$ space,

$$\tilde{\phi}(\mathbf{p})=h(p)Y_{lm}(\hat{\mathbf{p}}) \tag{A1}$$

is given by

$$(\tilde{V}_C\phi)(\mathbf{p})=I_l(p;h)Y_{lm}(\hat{\mathbf{p}}) , \tag{A2}$$

where

$$I_l(p;h)=-\frac{\gamma}{\pi p}\int_0^\infty dp'p'Q_l(z)h(p') . \tag{A3}$$

Here $Q_l(z)$ is the Legendre function of the second kind and $z=(p^2+p'^2)/2pp'$. We shall need the asymptotic behavior of I_l for $p\to\infty$, with $h(p)$ assumed to fall off as an inverse power of p:[10]

$$h(p)\sim C_h/p^{2+\nu} . \tag{A4}$$

To be precise, we assume that there exists a positive A such that $h(p)=(C_h/p^{2+\nu})[1+\mathcal{O}(p^{-1})]$ for $p\ge A$. We break up the integration range in (A3) into the intervals $(0,A)$ and (A,∞). In the first interval we may let $p\to\infty$ inside the integral and replace $Q_l(z)$ by its leading term for large z, viz., $Q_l\sim C_l z^{-l-1}$ and z by its value for large p, $z\sim p/2p'$, to get a contribution $I_l^{(1)}$ proportional to p^{-2-l}:

$$I_l^{(1)}(p;h)\sim\frac{\text{const}}{p^{2+l}} . \tag{A5}$$

From the second integral we get, using (A4), a contribution

$$I_l^{(2)}(p;h)\sim\frac{-\gamma C_h}{\pi p}\int_A^\infty\frac{dp'}{(p')^{1+\nu}}Q_l\left[\frac{p^2+p'^2}{2pp'}\right] . \tag{A6}$$

On setting $p'=py$ in (A6) and letting $p\to\infty$ we get

$$I_l^{(2)}(p;h)\sim\frac{-\gamma C_h}{\pi p^{1+\nu}}F_l(\nu) , \tag{A7}$$

where

$$F_l(\nu)=\int_0^\infty \frac{dy}{y^{1+\nu}}Q_l\left[\frac{1+y^2}{2y}\right] . \tag{A8}$$

From (A8) one finds that

$$F_0(\nu)=\frac{\pi}{\nu}\tan\frac{\pi\nu}{2} , \tag{A9}$$

and

$$F_1(\nu)=\frac{\pi\nu}{1-\nu^2}\cot\frac{\pi\nu}{2} , \tag{A10}$$

which are all that we will need.

2. Spin-0 equations

Consider an eigenvalue equation of the following generic form:

$$K(p)h(p)+L(p)I_l(p;h)=Wh(p) . \tag{A11}$$

For $K(p)=p^2/2m$ and $L(p)=1$, this is just the **p**-space Schrödinger equation for orbital angular momentum l. In this case, the leading term in $K(p)h(p)$ behaves as $p^{-\nu}$ for $p\to\infty$. This can only be balanced by $I_l^{(1)}(p;h)$, so that we must have $\nu=2+l$ or $h(p)\propto 1/p^{4+l}$ for large p, in agreement with the explicit solution, given, e.g., in the book of Bethe and Salpeter.[11]

Now suppose that $K(p)$ has the form of a relativistic kinetic energy, e.g.,

$$K(p)=(p^2+m^2)^{1/2}-m \tag{A12}$$

for the one-body problem, or

$$K(p)=(p^2+m_1^2)^{1/2}+(p^2+m_2^2)^{1/2}-m_1-m_2 \tag{A13}$$

for the two-body problem. Then for $p\to\infty$

$$K(p)\sim ap \quad (a=1 \text{ or } 2) \tag{A14}$$

and the leading term in $K(p)h(p)$ now behaves as $p^{-1-\nu}$. This can only be balanced by $I_l^{(2)}(p;h)$ so that we get the relation

$$\frac{a}{p^{1+\nu}}-\frac{\gamma}{\pi p^{1+\nu}}F_l(\nu)=0$$

or

$$\gamma(\nu)=\frac{\pi a}{F_l(\nu)} . \tag{A15}$$

In order that $h(p)$ be square integrable, with weight p^2, we need $\nu>-\frac{1}{2}$. Let $F_{l;\min}$ denote the minimum value of $F_l(\nu)$ in this region. Then we must have $\gamma<\gamma_{\max}$, where

$$\gamma_{\max}=\frac{\pi a}{F_{l;\min}} . \tag{A16}$$

3. Spin-$\frac{1}{2}$ equations

The treatment of these is a straightforward extension of the spin-0 case.

a. Dirac equation

We restrict ourselves to $j=\frac{1}{2}$ and positive parity. The coupled **p**-space equations for the wave functions $g(p)$ and $f(p)$, the Fourier-Bessel transforms of the usual radial functions, read

$$-pf(p)+I_0(p;g)=(E_D-m)g(p) ,$$

$$-pg(p)+I_1(p;f)=(E_D+m)f(p) .$$

With $g(p)\sim C_g/p^{2+\nu}$, $f(p)\sim C_f/p^{2+\nu}$ we get, using (A7)

$$-C_f-\frac{\gamma}{\pi}C_gF_0(\nu)=0 , \quad -C_g-\frac{\gamma}{\pi}C_fF_1(\nu)=0$$

which requires that

$$\gamma^2(\nu)=\frac{\pi^2}{F_0(\nu)F_1(\nu)}=1-\nu^2 . \tag{A17}$$

b. No-pair external-field equation

As shown in Ref. 2, $f(p)$ can be eliminated and the equation for $g(p)$ reads, for a $j=\frac{1}{2}$ state with positive parity,

$$E_1(p)g(p)-\frac{\gamma A_1(p)}{\pi p}\int_0^\infty dp'p'A_1(p')g(p')\times\left[Q_0(z)+\frac{p}{E_1(p)+m_1}\frac{p'}{E_1(p')+m_1}Q_1(z)\right]=E_+g(p) , \tag{A18}$$

where

$$A_1(p)=\{[E_1(p)+m_1]/2E_1(p)\}^{1/2} .$$

With $g(p)\sim C_g/p^{2+\nu}$ for large p, $A_1(p)\to 1/\sqrt{2}$ and (A18) leads to the condition

$$C_g-\frac{\gamma}{2\pi}[F_0(\nu)+F_1(\nu)]C_g=0$$

or

$$\gamma(\nu)=\frac{2\pi}{F_0(\nu)+F_1(\nu)} . \tag{A19}$$

c. h_{++} equation

(i) $V=V_C$. For a singlet $j=0$ state the relevant equation is now[12]

$$[E_1(p)+E_2(p)]g(p)-\frac{\gamma}{\pi}\int_0 k_0^{++}(p,p')g(p')p'^2dp'=E_{++}g(p) , \tag{A20}$$

where

$$k_0^{++}(p,p')=\frac{A(p)A(p')}{pp'}[(1+b_1b_2b_1'b_2')Q_0(z)+(b_1b_1'+b_2b_2')Q_1(z)]$$

with $b_i=p/(E_i+m_i)$, $b_i'=p'/(E_i'+m_i)$, and $A(p)=A_1(p)A_2(p)$. For large p, the b's$\to 1$, the A's$\to\frac{1}{2}$ so that we get, with $g \sim C_g / p^{2+\nu}$,

$$2C_g - \frac{\gamma}{\pi}\frac{1}{4}[2F_0(\nu)+2F_1(\nu)]C_g = 0$$

or

$$\gamma(\nu) = \frac{4\pi}{F_0(\nu)+F_1(\nu)} . \tag{A21}$$

(ii) $V = V_C + V_B$. The kernel k_0^{++} in (A20) gets replaced by

$$k_{0;B}^{++}(p,p') = \frac{A(p)A(p')}{pp'}[(1+b_1b_2b_1'b_2'+2b_1b_2 + 2b_1'b_2')Q_0(z) + (b_1b_1'+b_2b_2')Q_1(z)] .$$

For large p we then get

$$2C_g - \frac{\gamma}{\pi}\frac{1}{4}[6F_0(\nu)+2F_1(\nu)]C_g = 0$$

or

$$\gamma(\nu) = \frac{4\pi}{3F_0(\nu)+F_1(\nu)} . \tag{A22}$$

APPENDIX B: THE DIRAC EQUATION FOR $\alpha Z > 1$

As mentioned in Sec. I, the Dirac-Coulomb equation,

$$\left[\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m - \frac{\gamma}{r}\right]\psi(\mathbf{r}) = E_D\psi(\mathbf{r}) , \tag{B1}$$

has $\gamma \equiv \alpha Z = 1$ as a critical value in the sense that $E_D(1s)$ becomes imaginary for $\gamma > 1$. However, just precisely what it is that goes wrong at $\gamma = 1$ is not made entirely clear from a reading of the extant literature. The most comprehensive recent discussion of (B1) for large γ appears to be that in the book by Richtmyer,[5] where references to earlier work can be found. The purpose of this appendix is to extend that discussion, which we first briefly review.

1. Review

Let $\mathscr{D}$ denote the linear space of Dirac-spinor functions $\psi(x)$ and let $\mathscr{H}$ denote the subspace of square integrable ψ's:

$$\mathscr{H} = [\psi \mid \psi \in \mathscr{D}, \langle \psi \mid \psi \rangle < \infty] \tag{B2}$$

with

$$\langle \psi \mid \psi \rangle = \int d\mathbf{r}\, \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) . \tag{B3}$$

ψ's differing only on a set of measure zero are considered equivalent; $\mathscr{H}$ is then a Hilbert space. The domain of the free Dirac Hamiltonian h_D is defined by

$$D_0 = [\psi \mid \psi \in \mathscr{H}, \boldsymbol{\alpha}\cdot\nabla\psi \in \mathscr{H}] \tag{B4}$$

and h_D itself is defined as a linear mapping of D_0 into $\mathscr{H}$ with the property

$$h_D\colon \psi(\mathbf{r}) \to (h_D\psi)(\mathbf{r}) \equiv (\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m)\psi(\mathbf{r}) . \tag{B5}$$

It can be shown that D_0 is dense in $\mathscr{H}$ and h_D is self-adjoint on D_0.

Now let $T = T(\gamma)$ denote the linear-differential operator on the subspace of once-differentiable spinors in $\mathscr{D}$ defined by

$$T(\gamma)f(\mathbf{r}) = \left[\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m - \frac{\gamma}{r}\right]f(\mathbf{r}) . \tag{B6}$$

The attempt to define $H_{D;\text{ext}}$, with $V_{\text{ext}} = -\gamma/r$, as a self-adjoint linear operator on D_0, via

$$H_{D;\text{ext}}\colon \psi(\mathbf{r}) \to (H_{D;\text{ext}}\psi)(\mathbf{r}) \equiv T(\gamma)\psi(\mathbf{r}) , \quad \psi \in D_0 \tag{B7}$$

succeeds only for $\gamma < \gamma_* \equiv \sqrt{3}/2$. For $\gamma \geq \gamma_*$, the operator defined by (B7) is not self-adjoint on D_0. This is related to the fact that for $1 > \gamma \geq \gamma_*$ each of the usual normalizable solutions with $j = \frac{1}{2}$ of the equation

$$T(\gamma)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{B8}$$

is accompanied by another one for which, however, the expectation value of $V_C = -\gamma/r$ diverges. One is thus led to define the domain of $H_{D;\text{ext}}$ as

$$D = [\psi \mid \psi \in \mathscr{H}, T(\gamma)\psi \in \mathscr{H}, \langle \psi \mid V_C \mid \psi \rangle < \infty] , \tag{B9}$$

where

$$\langle \psi \mid V_C \mid \psi \rangle \equiv -\gamma \int d\mathbf{r}\, \psi^\dagger(\mathbf{r})\frac{1}{r}\psi(\mathbf{r}) . \tag{B10}$$

The linear operator $H_{D;\text{ext}}$ is then defined by

$$H_{D;\text{ext}}\colon \psi(\mathbf{r}) \to (H_{D;\text{ext}}\psi)(\mathbf{r}) \equiv T(\gamma)\psi(\mathbf{r}) , \quad \psi \in D . \tag{B11}$$

This limits the bound-state eigenfunctions of $H_{D;\text{ext}}$ to the usual ones. It is apparently still only a conjecture that for any $\gamma < 1$ the thus-defined $H_{D;\text{ext}}$ is self-adjoint on the domain D, which presumably is also dense in $\mathscr{H}$.

2. Remarks

The above discussion does not make it clear in just what way things go wrong for $\gamma \geq 1$, and it is to this question that we address ourselves. The fact that the function

$$E_D(1s) = (1-\gamma^2)^{1/2} m \tag{B12}$$

becomes complex when analytically continued to $\gamma > 1$ is not the end of the story. Let us first consider the eigenfunctions

$$\psi_{1s;\pm}(\mathbf{r};\gamma) \propto r^{-1 \pm (1-\gamma^2)^{1/2}} e^{-\gamma m r} \tag{B13}$$

associated with the eigenvalue (B12); an angle-dependent spinor-factor is suppressed. The function $\psi_{1s;-}$ is the one for which $\langle V_C \rangle = \infty$. It is readily verified that the analytic continuation of these functions to the region $\gamma > 1$ satisfy

$$T(\gamma)\psi_{1s;\pm}(\mathbf{r},\gamma) = \pm i(\gamma^2-1)^{1/2}\psi_{1s;\pm}(\mathbf{r};\gamma) . \tag{B14}$$

Thus as far as Eq. (B8) is concerned, nothing spectacular happens when γ exceeds unity. In particular, as is readily verified, both the functions $\psi_{1s;\pm}(\mathbf{r};\gamma)$ remain square integrable for $\gamma \geq 1$, contrary to what one might perhaps have guessed. The fact that the "Hermitian-looking" $T(\gamma)$ has complex eigenvalues for $\gamma > 1$ cannot therefore be associated with failure of normalizability of the $\psi_{1s;\pm}$ for $\gamma > 1$.

The key to understanding what is going on is to note that for $\gamma > 1$, *both* ψ's violate the condition

$$\langle \psi \mid V_C \mid \psi \rangle < \infty \ , \tag{B15}$$

so that neither belongs to D, and that the violation of this condition is directly connected with the possibility of complex values for E. To see this, note that if

$$T(\gamma)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (r \neq 0) \tag{B16}$$

and

$$\langle \psi \mid \psi \rangle \equiv \lim_{a\to 0} \int_{r \geq a} d\mathbf{r}\, \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) < \infty \ , \tag{B17}$$

we can set $\langle \psi \mid \psi \rangle = 1$ and, on multiplying (B16) by $\psi^\dagger(\mathbf{r})$ and integrating over $\mathbf{r}$, write

$$E = \lim_{a\to 0} \int_{r \geq a} d\mathbf{r}\, \psi^\dagger(\mathbf{r}) T(\gamma)\psi(\mathbf{r}) \ . \tag{B18}$$

Although for $\gamma > 1$ and $\psi = \psi_{1s;\pm}$, the kinetic and potential terms on the right-hand side of (B18) separately diverge as $a \to 0$, these divergences cancel in the sum. Now from (B18) we see that, for any real potential V,

$$E - E^* = \lim_{a\to 0} \int_{r \geq a} d\mathbf{r}[\psi^\dagger(\mathbf{r})\boldsymbol{\alpha}\cdot\mathbf{p}\psi(\mathbf{r}) - \text{c.c.}] \ . \tag{B19}$$

The integrand in (B19) can be rewritten as the divergence of $-i\psi^\dagger\boldsymbol{\alpha}\psi$ so that on use of Gauss' theorem one gets

$$E - E^* = \lim_{r\to 0} ir^2 \int d\Omega\, \psi^\dagger \boldsymbol{\alpha}\cdot\hat{\mathbf{r}}\psi \ . \tag{B20}$$

It follows that E is complex if and only if the integral in (B20) behaves precisely like $1/r^2$ for $r \to 0$. (If it were more singular, then E would be infinite.) Barring cancellations, this requires that

$$\psi \sim r^{-1} \tag{B21}$$

for $r \to 0$. This is, however, just sufficiently singular behavior to make $\langle V_C \rangle$ infinite. This establishes the claimed connection between complex values for E and the divergence of $\langle V_C \rangle$.

We can now return to the question of what happens to the operator $H_{D;\text{ext}}$, as defined by (B9) and (B11), for $\gamma > 1$. It is readily verified that H is symmetric (Hermitian) on the domain $D(H)$ defined by (B9) even when $\gamma > 1$, and it is plausible that $D(H)$ continues to be dense in $\mathscr{H}$ for $\gamma > 1$. But H is not self-adjoint because there exist vectors ϕ in $\mathscr{H}$ which satisfy $\langle \phi \mid T(\gamma)\psi \rangle = \langle T(\gamma)\phi \mid \psi \rangle$ for any $\psi \in D(H)$, but which do not belong to $D(H)$. An example is provided by the choice $\phi = \psi_{1s;+}(\mathbf{r};\gamma)$ given by (B13) with $\gamma > 1$, i.e., with $(1-\gamma^2)^{1/2} \equiv i \mid 1-\gamma \mid^{1/2}$. It follows that the domain $D(H^\dagger)$ of the adjoint $H^\dagger$ of H, defined as the set of all $\chi \in \mathscr{H}$ for each of which there exists a (unique) vector $\chi' \equiv H^\dagger \chi$ with the property that $\langle \chi \mid T(\gamma)\psi \rangle = \langle \chi' \mid \psi \rangle$ for all $\psi \in D(H)$, is larger than $D(H)$. Thus, a vital aspect of the definition of self-adjointness, the equality of $D(H)$ and $D(H^\dagger)$, is not satisfied. Moreover, $H^\dagger$ is not symmetric, so that H also cannot be essentially self-adjoint.

As a final point, the reader may be wondering whether the function $\psi_{1s;-}(\mathbf{r};\gamma)$ does not provide a counter example to our explication of the connection between the divergence of $\langle V_C \rangle$ and the existence of complex eigenvalues for $T(\gamma)$ when $\gamma > 1$. After all, for $\sqrt{3}/2 < \gamma < 1$, the quantity $\langle \psi_{1s;-} \mid V_C \mid \psi_{1s;-} \rangle$ is infinite but, nevertheless, the associated energy E is real. The answer to this lies in the phrase "barring cancellations" used in our discussion above. It is easy to verify that the functions

$$F_\pm(\mathbf{r};\gamma) = \psi^\dagger_{1s;\pm}(\mathbf{r};\gamma)\boldsymbol{\alpha}\cdot\hat{\mathbf{r}}\psi_{1s;\pm}(\mathbf{r};\gamma) \tag{B22}$$

vanish for $\gamma < 1$, because of a cancellation between the cross-terms arising from the mixing of the upper and lower components of ψ with the lower and upper components of $\psi^\dagger$, respectively. Thus for $\gamma < 1$ the integrand on the right-hand side of (B20) vanishes for both $\psi_{1s;+}$ and $\psi_{1s;-}$ and there is, in particular, no constraint on the behavior of $\psi_{1s;-}$ as $r \to 0$. However, because of the complex conjugation involved in (B22), the functions $F_\pm$ are not analytic functions of γ. Hence they can be and indeed are nonvanishing for $\gamma > 1$, consistent with the fact that E is complex in this region. A nice feature of (B20) is that it expresses the imaginary part of E directly in terms of the wave function at the origin, where lies the source of both the Coulomb potential and the troubles for $\gamma > 1$.

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[1]For recent reviews, see, e.g., W. Greiner, in *Proceedings of the International Conference on Nuclear Physics, Florence, 1983*, edited by P. Blasi and R. A. Ricci (Tipografia Compositori, Bologna, 1983), p. 635; J. Rafelski, L. P. Fulcher, and A. Klein, Phys. Rep. **38C**, 228 (1978); S. J. Brodsky and P. J. Mohr, in *Structure and Collisions of Ions and Atoms,* edited by I. A. Sellin (Springer, Berlin, 1978), p. 3.

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[12]Equation (A20) follows from Eqs. (3.4) and (3.6) of Ref. 2 on specializing to a $^1S_0$ state.