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STRONGLY COUPLED POSITRONIUM: SOLUTION METHODS AND POTENTIALS

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CHAPTER 1

INTRODUCTION

Physics students learning quantum mechanics use the Schrödinger equation to study the hydrogen atom. A solution of the Schrödinger equation consists in finding all energies and corresponding wave functions. The energy spectrum determines the spectrum for optical transitions which can be compared to experiment. This correspondence between theoretical prediction and experiment determines the degree of validity or applicability of the Schrödinger equation. In a similar way, this thesis applies an equation from relativistic quantum mechanics to positronium. The applicability of the equation is determined by its predictions.

Positronium is the bound state of the electron and its antiparticle, the positron. It is a two-particle system like the hydrogen atom and, in fact, it is sometimes referred to as the positronium atom. As in the case of the hydrogen atom, the Coulomb potential is responsible for the interaction between the constituent charged particles. In this thesis, however, and in addition to the fact that the equation and constituent particles are different, two major differences from the textbook study of hydrogen are significant. These differences are that in the Coulomb potential, expressed in natural units ($\hbar = c = 1$) as $-\alpha/r$, the fine structure constant α, where $\alpha = e^2/\hbar c$, or e^2 in natural units, is allowed to increase from its physical value of about 1/137, and that the Coulomb potential is truncated in order to avoid its non-physical singularity at the origin. Chapters 3 and 4 are concerned with the significance of varying α, while the truncating of the Coulomb potential, in addition to its importance in Chapters 3 and 4, leads to Chapters 5 through 8 which are on the subject of matching of the constants as a method of finding exactly solvable potentials in the radial Schrödinger and Klein-Gordon equations.

1-1 Defining positronium. Positronium (Ps) is the bound state of the electron and the positron. The electron and positron carry opposite charges and thus are subject to the Coulomb force. Unlike the proton and the electron of hydrogen, however, the electron and the positron of positronium have equal mass. This last fact is used to make a comparison of the Bohr radius of the two atoms. Given that the reduced mass, μ, for a system of two masses, m_1 and m_2, is

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{1-1}$$

it can be shown that the reduced mass of hydrogen is approximately equal to the mass of the electron, while the reduced mass of positronium is exactly half the mass of the electron. Finally, recalling that the Bohr radius, written in CGS units, is

$$a_0 = \frac{\hbar^2}{\mu Z e^2} \tag{1-2}$$

and noting that the Bohr radius is inversely proportional to the reduced mass, we see that the Bohr radius of positronium is about twice that of hydrogen.

Though positronium is not as common as hydrogen, it is an atom that can be produced in the lab. Positronium production is described by Werth (Bassani, 1989, pp. 161-170) and relies on collisions of low energy positrons in gases or on surfaces. To fill in one detail of interest in positronium production, the conventional source of the positrons are the radioactive positron emitters ^{22}Na or ^{58}Co. Werth also states that, as of 1989, experimental knowledge of positronium was limited to atomic states of principal quantum numbers of $n = 1$ and $n = 2$ (Bassani, 1989, p. 161). This limitation is mentioned as a note of interest in positronium research and is not meant to be taken as a barrier to this work since our interest here is in the $n = 1$ atomic state.

In fact, the specific atomic state of positronium that we study is the ground state of parapositronium, where the prefix "para" indicates that the net spin of the electron positron system is zero. Using the notation $n^{2S+1}L_J$, this atomic state of positronium is given as 1^1S_0, or more simply as the ^{1}S$_0$ state, keeping in mind that $n = 1$.

There is also an "orthopositronium," a name indicating that the net intrinsic spin of the electron plus the positron of positronium is one. Orthopositronium decays into three photons since there is no way that two photons can have a net spin of one, recalling that photons have spin ± 1. On the other hand, parapositronium decays into two photons, such that the two photons move in opposite directions and the spins cancel. The lifetime of orthopositronium, due to its more complicated decay mode, is longer than that of parapositronium. Referring to the ground state, the theoretical lifetimes are 1.4208 x 10^{-7} seconds for orthopositronium, and 1.2525 x 10^{-10} for parapositronium (Bassani, 1989, p. 161).

That the decay modes of positronium is being discussed in the first place is due to the fact that matter (the electron in this case) combined with anti-matter (the positron) annihilate each other. Matter annihilation is a relativistic phenomenon, made possible by $E = mc^2$; hence, to incorporate relativity into the mathematical description of positronium, we need to use a relativistic quantum mechanical equation. The Schrödinger equation will not suffice, at least when the energies become comparable to the rest masses. Furthermore, since two-body relativistic wave equations are still very much an open area of research (Landau, 1990, p. 219), our primary focus in this thesis is actually a particular two-particle wave equation and not positronium. Positronium just happens to be a clean and relatively simple physical system with which to study this equation.

1-2 Why positronium? An important difference between positronium and hydrogen is that the electron and the positron of positronium are leptons. In contrast, the proton of hydrogen is not a lepton and is subject to the strong force, thus marring the spectrum of hydrogen with uncertainties and making the comparison between experiment and theory more difficult. On the other hand, positronium is an ideal system on which to apply the theory of quantum electrodynamics. Specifically, concerning positronium, "the only significant interaction present at current levels of experimental and calculational precision between the positron and electron is the electromagnetic interaction. This feature has made Ps a sensitive testing ground for the theory of quantum electrodynamics (QED), in particular, its formulation in the relativistic two-body equation as embodied by the Bethe-Salpeter equation" (Nico, 1990).

In this thesis, however, a quantum field theoretical treatment of positronium is not the focus. We remain within the framework of wave equations and wave functions with their single particle charge density interpretation, in which the negative-energy solutions are reinterpreted in the Dirac sea and hole picture. These negative-energy solutions play a crucial role in the study of annihilation and the lifetime of positronium, and they need to be considered when determining physical values of the constants.

The lifetime of positronium, particularly the lifetime of orthopositronium, is an important subject of research because of the small discrepancy that currently exists between theory and experiment and which could indicate trouble for QED (Kinoshita, 1990, p. 10); however, that issue does not concern us here. This research is not concerned with the decay rate of positronium, but with the decay of the vacuum (Greiner, 1985). In particular, strongly bound positronium, obtained by mathematically increasing the fine structure constant, is being modeled with a two-particle relativistic wave equation for the purpose of

predicting stability or instability with regard to real electron-positron pair creation. Comparisons can be made with the corresponding predictions of stability from other wave equations, ultimately for the purpose of knowing which of the equations agree with experiment.

Looming in the background, but beyond the scope of this thesis, is the interest in strong Coulomb fields and positronium for insight that may be gained in QED and quantum chromodynamics (QCD) research (Bawin, 1990). In particular, heavy-ion experiments have led to the conjecture of a new phase of QED in sufficiently strong Coulomb fields (Fried, 1991, pp. 195-221). The overlap of this research and QCD can be seen in the fact that positronium is similar to quarkonium inasmuch as both atoms are a bound state of two equal mass, particle-antiparticle, fermionic (half-integer) particles. Therefore, a two-particle relativistic wave equation that is appropriate for the positronium would be applicable to quarkonium. In addition, although the interaction in quarkonium is different from the interaction in positronium, recalling that there are no free quarks, a Coulomb type potential may dominate at shorter distances (Fabiano, 1994); thus insight into short distance QCD may be gained.

1-3 The interaction. In natural units the Coulomb potential for positronium is written as $-\alpha/r$, where α is the fine structure constant and represents the strength of the interaction. In this work, α is allowed to increase from its physical value of about 1/137 to ∞, and thus, a strong Coulomb field is produced. In a strong Coulomb field, positronium is referred to as "strongly coupled positronium," a term used in succeeding chapters. A difference between this mathematical exercise and heavy-ion experiments is that the factor α is increased instead of Z in the formula $-Z\alpha/r$; ($Z = 1$ for positronium). In either case, comparable strong Coulomb fields can be achieved via the $Z\alpha$ term of the equation. In addition, one reason why we do not go beyond $\alpha = 1.5$ is that this value of α corresponds to a heavy-ion having 205 protons. Incidentally, a second reason for not going beyond $\alpha = 1.5$ is that, according to our present understanding of Quantum Electrodynamics of strong fields, production of electron-positron pairs is expected to occur in the external Coulomb field of a nucleus of charge Z when Z exceeds a critical value of 170 (Greiner, 1985). Therefore, extrapolating to positronium, we may expect to find stability or instability with respect to spontaneous production of bound electron-positron pairs, according to the equation that we use, to indicate itself without having to go beyond $\alpha = 1.3$.

Increasing α affects the total energy of strongly coupled positronium because the charged constituent particles become more tightly bound in a stronger field. In particular, the energy is found according to the two-particle relativistic wave equation that is being used, as a function of field strength, to see if there is a critical value of α, beyond which the value of the energy indicates instability of strongly coupled positronium with regard to spontaneous electron-positron pair creation. If no such α is found, then the implication is stability of spontaneous pair production.

In playing the game of increasing α, however, it is necessary to truncate, or regularize, the Coulomb potential for another reason in addition to that of avoiding the non-physical singularity at $r = 0$. Recall that regularization of the Coulomb potential is required when a Klein-Gordon particle is in a strong field such that $Z\alpha > 1/2$ to avoid loss of self-adjointness, as discussed by Case (1950). In the case of a Dirac particle, regularization of the Coulomb potential is needed for $Z\alpha > 1$. Since the equation that is used in succeeding chapters to describe strongly coupled positronium which is formally identical to the S-wave radial Klein-Gordon equation, and since we have $Z = 1$, regularization of the Coulomb potential will be necessary for us to go beyond $\alpha = 1/2$.

In a recent paper by Bawin and Cugnon (Bawin, 1990), the same two-particle wave equation (specifically Eq. (2-17) as it is introduced in Chapter 2) that will be used in Chapters 3 and 4 of this work predicted stability for all finite values of α. Bawin and Cugnon's prediction was made using the following regularized Coulomb potential, namely

$$V(r) = \frac{-\alpha}{r} \qquad (r > r_0) \tag{1-3}$$

$$V(r) = \frac{-\alpha}{r_0} \qquad (r < r_0) \tag{1-4}$$

where r_0 is an arbitrarily small cut-off radius. The constant potential in the domain $r < r_0$ avoids the non-physical singularity of the Coulomb potential at $r = 0$, and corresponds to the potential of a spherical conductor of radius r_0 with uniform charge distribution on its surface.

After recovering Bawin and Cugnon's prediction of stability as part of the discussion of Chapter 3, a result that is in sharp contrast to the corresponding predictions from the Dirac and Klein-Gordon equation (Bawin, 1990), the potential given by Eqs. (1-3) and (1-4) is replaced by the following potential:

$$V(r) = \frac{-\alpha}{r} \qquad (r > r_0) \tag{1-3}$$

$$V(r) = \frac{3\alpha}{2r_0^3}\left[\frac{r^2}{3} - r_0^2\right] \qquad (r < r_0) \tag{1-5}$$

as the subject of Chapter 4. Once again, r_0 is an arbitrarily small cut-off radius. The singularity of the Coulomb potential at $r = 0$ is now avoided with a quadratic potential in the domain $r < r_0$. The quadratic potential, Eq. (1-5), corresponds to a sphere of radius r_0 with a uniform charge distribution throughout its volume. As such, this model may be more physical than the previous model of an electron that has a surface charge distribution because of the precedent that the nucleus has a fairly uniform charge distribution. In addition, Eq. (1-5) has a continuous first derivative and therefore it represents a continuous electric field, unlike the potential energy of Eq. (1-4).

None of the arguments for a particular model should be taken too literally, however. We know that the electron or positron has no spatial structure above 10^{-18} meters, and that nothing is known about spatial structure below this value. Classical prescriptions for charge distribution models have problems from the point of view of relativity (rigidity, crossing the speed of light) and from the point of view of quantum mechanics (trajectory, interpretation of probability density). Therefore, the potentials themselves should be interpreted as exhibiting some structure which could arise from quantum field theoretical calculations. Wave equations with potentials are used here as a first step to understanding more sophisticated theories.

The use of different truncations of the Coulomb potential should be viewed as a test for the consistency of the theory behind the equation being used. In fact, for either choice of truncating potential, the electron is modeled as a point charge in the limit as $r_0 \to 0$, and therefore it is expected that the prediction of stability or instability will be independent of the choice of truncation. If different results for different models of the electron are found, then this may be considered as a weakness of the approach behind the equation rather than a final statement about a particular potential. In short, this thesis compares the prediction of stability or instability from a two-particle wave equation with respect to spontaneous electron-positron pair creation, depending on which of the two truncating potentials is used in the equation.

1-4 Matching of the constants. Details of the two-particle relativistic equation that is used in this work have not, as yet, been given (they are found in Chapter 2). Thus, information discussed up to this point could be applied to any one of the many two-particle wave equations available in the literature—a degree of freedom that opens a door to future research. Before a second topic of this thesis is introduced, however, it is necessary to mention that the equation to be used is formally identical to the S-wave radial Klein-Gordon.

In the course of studying the two-particle wave equation with the potential of Eq. (1-3) and (1-5), we were led to consider methods of finding exactly solvable potentials in homogeneous, second-order, linear differential equations. In particular, methods of finding exactly solvable potentials became an area of interest as the quadratic truncating potential of Eq. (1-5) was substituted into the formally identical S-wave radial Klein-Gordon wave equation and then solved using Frobenius' method. As will be seen in Chapter 4, Frobenius' method yields expressions for which convergence is difficult to ascertain and for which the solutions must be approximated in keeping the first few terms of the infinite series. Finding a closed form solution, or even searching for other truncating potentials with closed form solutions, led to an alternative method of solving the wave equation besides assuming a power series solution. One method that was particularly attractive to us for finding exactly solvable potentials was the method of "matching of the constants" (Beker, 1993).

In the method of matching of the constants, a differential equation with a known solution is transformed by replacing the independent variable of the equation's solution with an unspecified function of a new independent variable and then changing independent variables of the differential equation to the independent variable of that function. Terms of the transformed differential equation's invariant function (Birkhoff, 1978, p. 46) are then matched with terms of the wave equation's invariant function, both equations having the same independent variable. The generality of the method is that the function that is the original independent variable of the differential equation is unspecified and is selected to yield a constant term in the transformed equation's invariant function such that this term can be matched with the constant energy term in the invariant function of the wave equation. Successful matching of the remaining terms derives expressions for the potential energy and the energy.

Matching of the constants is backwards from the usual process of solving wave equations in the sense that the solutions, in closed form, are assumed from the start, and it is the potential that is derived, as opposed to substituting a known potential into the wave

equation and then deriving the solutions. Matching of the constants amounts to a solution begging for a problem.

The method of matching of the constants shall be used here to derive exactly solvable potentials in the radial Schrödinger and Klein-Gordon equations. The Schrödinger equation is used to demonstrate and practice the method on familiar grounds, while the radial Klein-Gordon equation is used to tie in matching of the constant with the research on strongly coupled positronium. Although we did not foresee matching of the constants from the outset of this research, developing techniques to find exactly solvable potentials is an important area of research in itself. For example, perturbation theory in quantum mechanics relies on having potentials with closed form solutions. In the very least, the chapters on matching of the constants provide an alternative to Frobenius' method for obtaining solutions corresponding with well known potentials and they provide a review of other potentials found in the literature.

1-5 Overview. Chapter 2 reviews relativistic wave equations beginning with the Klein-Gordon and the Dirac equations, leading to a presentation of the two-body wave equation that we use to study strongly coupled positronium. In Chapter 3, we solve this equation with the truncated Coulomb potential of Eqs. (1-3) and (1-4). A transcendental equation is derived by matching the logarithmic derivatives of the two solutions at the boundary of the two domains, from which the energy of strongly coupled positronium as a function of α is found numerically. Data tables are placed at the end of this thesis along with a plot of the data.

In Chapter 4, Frobenius' method, (not used in Chapter 3) is used to solve the wave equation now using the potential of Eqs. (1-3) and (1-5). The physical solution that is found corresponding to the quadratic potential of Eq. (1-5) is approximated by keeping the first term of the power series solution. We also return to this point two more times and keep the first two terms and then the first three terms of the solution. A new transcendental equation is obtained but the algebraic results of Chapter 3 are again useful in finding the energy of strongly coupled positronium as a function of α. Data tables and plots of the data pertaining to each of the three approximations of the solution in the $r < r_0$ domain are found at the end of the thesis.

Chapter 5 is a change of topics from strongly coupled positronium to matching of the constants as a method of deriving exactly solvable potentials. Matching of the constants is mathematically introduced and illustrated. Chapter 6 applies the method of matching of the constants starting with the confluent hypergeometric differential equation to derive three

exactly solvable potentials in the radial Schrödinger equation. Chapter 7 features the hypergeometric equation and the radial Schrödinger equation. Three more potentials are derived. Chapter 8 looks for exactly solvable potentials in the radial Klein-Gordon equation. Chapter 9 offers a conclusion to this work.

CHAPTER 2

RELATIVISTIC WAVE EQUATIONS

The Klein-Gordon and Dirac equations are two well-known relativistic equations appropriate for spinless and spin-$\frac{1}{2}$ particles, respectively. Both of these one-particle equations are also relevant to this work. The Dirac equation appears in the derivation of the two-particle equation that is used here, which turns out to be an equation formally identical to the S-wave radial Klein-Gordon equation. Therefore, both equations are introduced in this chapter. Also introduced is the two-particle equation which will be solved later in Chapters 3 and 4 in connection with this study of strongly coupled positronium.

The two-particle equation we use is due to H. W. Crater and P. Van Alstine and derived in the framework of relativistic constraint dynamics (Crater, 1987). Roughly speaking, because in a relativistic two-body problem there is not an absolute time, changing to relative and center-of-momentum coordinates is not a textbook procedure as it is in the non-relativistic two-particle problem. Crater and Van Alstine's approach to deriving their two-particle wave equation, however, has "seemed to reopen the door to manifestly covariant (this time full four vector) canonical (in relativistic phase space) quantized descriptions" (Crater, 1994). The "door" that is being referred to pertains to the difficulties that arise in insisting that "relativistic interactions among point particles be realized canonically with a common parametric time chosen as the time for each particle" (Crater, 1994).

One reason for trusting the Crater and Van Alstine equation is that a closed-form energy spectrum is obtained that is in agreement with that of parapositronium through order α^4 (Crater, 1987). Another reason is that the Crater and Van Alstine equations correctly reduce to the Dirac equation (with a Coulomb interaction) when one of the particle masses becomes infinite (Bawin, 1990). On the other hand, since two-particle wave equations are still an open area of research (Landau, 1990, p. 219), our goal here is to test the validity of the Crater and Van Alstine two-particle equation, based upon the consistency or inconsistency of its prediction of the strong field behavior of the energy of positronium, for two different potentials.

2-1 Klein-Gordon equation. The Klein-Gordon equation is a relativistic quantum mechanical equation appropriate for spinless particles. It can be derived (using natural units, $\hbar = c = 1$) through the substitution of $i\partial/\partial t$ in place of E and $-i\nabla$ in place of p in the relativistic energy-momentum formula $E^2 = p^2 + m^2$. In an external electromagnetic field, through a relativistic application of minimal electromagnetic coupling, it becomes

$$\left(i\frac{\partial}{\partial t} - q\Phi\right)^2 \Psi(\mathbf{x},t) = \left[\left(\frac{\nabla}{i} - q\mathbf{A}\right)^2 + m^2\right]\Psi(\mathbf{x},t) \tag{2-1}$$

where $\mathbf{A}$ is a vector potential and Φ is a potential that transforms like the time component of a 4-vector, and is referred to as the "scalar" potential. In all applications of Eq. (2-1) throughout this thesis, it will turn out that $q\mathbf{A} = 0$, a fact that simplifies the equation.

Another simplifying fact is that only an S-wave radial Klein-Gordon type equation is needed for parapositronium. Therefore, the S-wave radial Klein-Gordon equation is now derived from Eq. (2-1). Based on the potentials that we will be using (as introduced in Chapter 1), the first step of the derivation is to set $q\mathbf{A} = 0$, and $q\Phi = V(r)$ in Eq. (2-1). Next, using spherical coordinates, the method of separation of variables is initiated by assuming a solution of the form

$$\Psi(\mathbf{x},t) = \frac{u_l(r)}{r} Y_{lm}(\theta,\phi) e^{-iEt} \tag{2-2}$$

Equation (2-2) is now substituted into and differentially operated on by Eq. (2-1), as follows.

The right-hand side of Eq. (2-1), after setting $q\mathbf{A} = 0$, has become

$$\left(-\nabla^2 + m^2\right)\Psi \tag{2-3}$$

The expression of the Laplacian, in spherical coordinates, is

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}L^2 \tag{2-4a}$$

where L^2, the angular momentum squared, is

$$L^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial^2\phi} \tag{2-4b}$$

The first term of Eq. (2-4a) takes derivatives with respect to r only. Indicating the number of derivatives taken with respect to r with primes, the first term only of Eq. (2-4a) operating on Ψ, leads to

$$-\frac{u_\ell''}{r}Y_{\ell m}(\theta,\phi)e^{-iEt} \tag{2-5}$$

while the second term of Eq. (2-4a), with L^2 given in Eq. (2-4b), operating on Ψ, leads to

$$\frac{\ell(\ell+1)u_\ell}{r^3}Y_{\ell m}(\theta,\phi)e^{-iEt} \tag{2-6}$$

Adding Eqs. (2-5) and (2-6) and remembering to include the m^2 of Eq. (2-3), the right-hand side of the Klein-Gordon equation, Eq. (2-1) becomes

$$\left\{-\frac{u_\ell''}{r}+\left[\frac{\ell(\ell+1)}{r^2}+m^2\right]\frac{u_\ell}{r}\right\}Y_{\ell m}(\theta,\phi)e^{-iEt} \tag{2-7}$$

Turning our attention to the left-hand side of Eq. (2-1), the end result of operating on Ψ is expressed as

$$(E-V)^2\frac{u_\ell}{r}Y_{\ell m}(\theta,\phi)e^{-iEt} \tag{2-8}$$

Equating the left-hand side to the right-hand side, or Eq. (2-8) to Eq. (2-7), and using the fact that the $Y_{\ell m}(\theta,\phi)e^{-iEt}$ form a complete set of independent functions, the radial Klein-Gordon equation is obtained:

$$u_\ell''+\left[(E-V)^2-\frac{\ell(\ell+1)}{r^2}-m^2\right]u_\ell = 0 \tag{2-9}$$

Finally, setting $\ell = 0$ in Eq. (2-9), the centrifugal barrier disappears and the S-wave radial Klein-Gordon equation becomes

$$u'' + \left[(E-V)^2 - m^2\right]u = 0 \tag{2-10}$$

Solutions of Eq. (2-10) will be studied in Chapters 3, 4, and 8. Our immediate attention is now turned to the Dirac equation.

2-2 Dirac equation. The Dirac equation is a relativistic wave equation that is used to describe spin-$\frac{1}{2}$ particles, such as the electron, and the positron. In fact, the Dirac equation is important historically because the positron was first predicted from this equation.

The Dirac equation, for a free particle of mass m, in covariant form, is

$$\gamma^\mu p_\mu \Psi(\mathbf{x},t) = m\Psi(\mathbf{x},t) \tag{2-11}$$

where summation over the Greek index is implied $(\mu = 0,1,2,3)$, the Dirac γ matrices are found in Landau (1990, p. 246), and

$$p_\mu = i\left(\frac{\partial}{\partial x^\mu}\right) = i\left(\frac{\partial}{\partial t}, \nabla\right) \tag{2-12}$$

Thus, remaining in natural units, and rearranging slightly, Eq. (2-11) becomes

$$\left(\gamma^\mu p_\mu - m\right)\Psi = 0 \tag{2-13}$$

Prior to writing the Klein-Gordon equation in Eq. (2-1), minimal electromagnetic coupling was invoked in order to describe a particle in an external electromagnetic field. That step is followed here by substituting

$$p^\mu \rightarrow p^\mu - qA^\mu \tag{2-14}$$

into the free particle Dirac equation of Eq. (2-13), where $A^\mu = (\Phi, \mathbf{A})$, a four vector consisting of the scalar and vector potentials, leading to

$$\left[\gamma^\mu\left(p_\mu - qA_\mu\right) - m\right]\Psi = 0 \tag{2-15}$$

Our need for Eq. (2-15) is minimal, but the equation is included in this chapter for the following two reasons. First, two coupled Dirac equations appear at the outset of the derivation that leads to the two-particle wave equation used here (Van Alstine, 1986). Thus, we need to be familiar with the Dirac equation to introduce the next section. Second, the Dirac equation has been used to describe an electron in the external Coulomb field of a nucleus of charge Z, and predicts the occurrence of spontaneous electron positron pair creation beyond $Z \approx 172$. This problem is found in Greiner (1985), from which Fig. 2-1 and Table 2-1 is taken. We note that the truncating potential that Greiner uses is that of a homogeneously charged sphere—our truncating potential of Eq. (1-5). Therefore, although we are using a two-particle equal mass wave equation for strongly coupled positronium, we might be biased to also find instability in this work at a corresponding value of $\alpha \approx 1.25$. Conversely, since the Crater and Van Alstine equations reduce to the Dirac equation when the mass of one of the particles becomes infinite, not finding instability may be a difference in the strong field behavior of an equal mass system compared with the unequal mass case (Bawin, 1990).

2-3 The Crater and Van Alstine equation. Crater and Van Alstine have recently applied Dirac's constraint dynamics and supersymmetry to a system of two spinning particles to derive two coupled Dirac equations that govern the quantum mechanics of two spin-$\frac{1}{2}$ particles interacting through world scalar and vector potentials (Crater, 1987). For the specific case of electromagnetic structure, minimal substitutions are made into free Dirac equations, such that $p_1 \rightarrow p_1 - A_1 \equiv \pi_1$ and $p_2 \rightarrow p_2 - A_2 \equiv \pi_2$, leading to two coupled Dirac equations written as

$$\gamma_1^5(\pi_1 \cdot \gamma_1 + m_1)\psi = 0 \tag{2-16a}$$

$$\gamma_2^5(\pi_2 \cdot \gamma_2 + m_2)\psi = 0 \tag{2-16b}$$

where a chiral Dirac matrix representation is being used. As luck would have it, Crater and Van Alstine use the convention of a plus in front of the mass instead of a minus sign as written in Eq. (2-13). This difference in sign convention should not slow us down at this point, however, because only m^2 terms appear in the two-particle equation, as will be noted presently. Also in anticipation of things to come, we note for future reference that

$A_1 = A_2 = (q\Phi, q\mathbf{A}) = (V(r), 0)$, where $V(r)$ is the potential energy term describing the electromagnetic interaction.

Setting these two equations aside momentarily, a list of the kinematic variables relevant to the constraint description of the relativistic two-body problem, found in Crater (1983), is now given here for the case of $m_1 = m_2 = m$:

(i) relative position, $x_1 - x_2$

(ii) relative momentum, $p = \frac{1}{2}(p_1 - p_2)$

(iii) total c.m. energy, $W = \sqrt{-P^2}$

(iv) total momentum, $P = p_1 + p_2$

(v) constituent c.m. energies, $\varepsilon_1 = \varepsilon_2 = W/2$

(vi) relativistic reduced mass and energy of the fictitious particle of relative motion,

$$m_W = \frac{m^2}{W} \qquad \varepsilon_W = \frac{W^2 - 2m^2}{2W}$$

In these expressions, x, p and P are 4-vectors and P^2 is negative.

Returning to the two coupled Dirac equations above, a rough outline of how these equations, in the c.m. frame, reduce to an equation that is formally identical to the S-wave radial Klein-Gordon equation is now given. Mathematical details, which are not the focus of this thesis, can be found in Van Alstine (1986). To begin, Eqs. (2-16a) and (2-16b) are "squared" and then the two resulting equations are subtracted and added together. The difference equation is equivalent to $2P \cdot p\psi = 0$ a condition that removes the relative time in the center-of-mass rest frame, while the summed equation divided by two leads to an equation that collapses for an *equal-mass singlet wave function* ϕ_S into the following equation:

$$\left[\mathbf{p}^2 + m_W^2 - (\varepsilon_W - V)^2\right]\varphi = 0 \tag{2-17}$$

The parameters ε_W and m_W have been defined above in (vi), but for convenience, they will be referred to later with the following equations numbers:

$$\varepsilon_W = \frac{W^2 - 2m^2}{2W} \tag{2-18}$$

$$m_W = \frac{m^2}{W} \tag{2-19}$$

For convenience in anticipation of solving Eq. (2-17), this equation is now put into the invariant form of differential equations, as described by Birkhoff (1978, p. 46). Using spherical coordinates, the differential momentum operator $-i\nabla$ replaces $\mathbf{p}$, and, keeping in mind that for the ${}^1S_0$ state we have $\varphi = \varphi(r)$, the following variable switch is made in Eq. (2-17),

$$\varphi(r) = \frac{u(r)}{r} \tag{2-20}$$

leading to

$$\frac{d^2u}{dr^2} + \left[\left(\varepsilon_W - V\right)^2 - m_W^2\right] u(r) = 0 \tag{2-21}$$

Finally, note that Eq. (2-21), when compared with Eq. (2-10), is an equation that is formally identical to the S-wave radial Klein-Gordon equation, where E, the energy of a Klein-Gordon particle in Eq. (2-10), is analogous to ε_W, the reduced energy of the fictitious particle of relative motion in this relativistic two-particle application, and m in Eq. (2-10), the mass of a Klein-Gordon particle, is analogous to m_W, the reduced mass of the fictitious particle in the two-particle problem. Equation (2-21) will be solved presently, for the truncated Coulomb potential of Eqs. (1-3) and (1-4), with the purpose of obtaining $W/2m$ as a function of α to determine whether there is an α beyond which $W/2m$ becomes negative.

FIG. 2-1. Instability of the Dirac equation in a strong field (Greiner, 1985, p. 85).

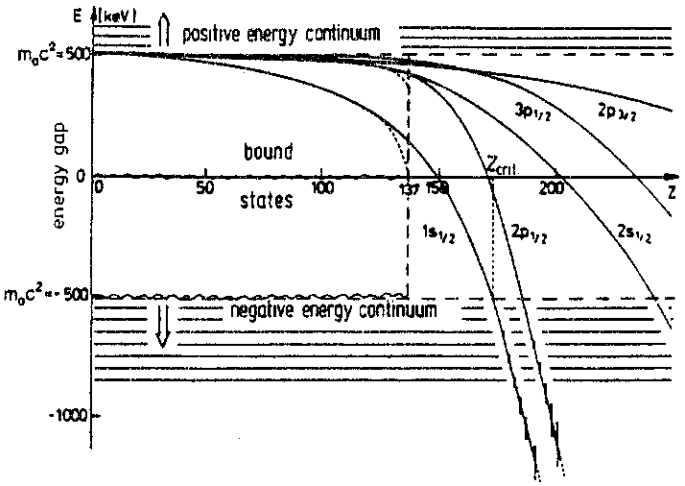


Fig. 3.14. Energies of the Dirac equation for an electron in a Coulomb-central field. The dots indicate the energies for point nuclei (fine-structure formula), which exist for $s_{1/2}$ and $p_{1/2}$ states only up to $Z = 137$. (———) represent the energies for extended nuclei. The overcritical case ($Z > Z_{crit} \approx 172$) is discussed in Chap. 6 [Mü 72b]

TABLE 2-1. Binding energies of the Dirac equation in a strong field (Greiner, 1985, p. 85).

Table 3.3. The binding energies of $1s_{1/2}$ electrons in keV as a function of the central charge Z. The energies assuming a point nucleus (Sommerfeld's fine structure formula) are compared with results for extended nuclei. For this calculation the potential of a homogeneously charged sphere with radius $R = 1.2A^{1/3}$ fm and $A = 2.5Z$ was used

Z	E_b^{point}	E_b^{ext}	Z	E_b^{point}	E_b^{ext}
10	− 1.362	− 1.362	100	−161.615	− 161.166
20	− 5.472	− 5.472	110	−206.256	− 204.890
30	− 12.396	− 12.395	120	−264.246	− 259.693
40	− 22.254	− 22.253	130	−349.368	− 330.749
50	− 35.229	− 35.227	137	−499.288	− 394.741
60	− 51.585	− 51.578	140	−	− 427.012
70	− 71.699	− 71.679	150	−	− 563.062
80	− 96.117	− 96.062	160	−	− 758.490
90	−125.657	−125.502	169	−	−1001.154

CHAPTER 3

STRONGLY COUPLED POSITRONIUM

Strongly coupled positronium in the ${}^1S_0$ state is studied using an equation that is formally identical to the S-wave radial Klein-Gordon. This equation is presently solved for a truncated Coulomb potential leading to a transcendental equation that contains the center-of-mass energy. The numerical solution of the transcendental equation highlights this chapter, as the center-of-momentum energy of the ${}^1S_0$ state of strongly coupled positronium is found as a function of the coupling constant α. Finally, the prediction of stability or instability from the Crater and Van Alstine equation is observed. Natural units with $\hbar = c = 1$ are used.

3-1 Solving the differential equation. We now solve Eq. (2-21)

$$\frac{d^2u}{dr^2} + \left[\left(\varepsilon_W - V\right)^2 - m_W^2\right] u(r) = 0 \tag{2-21}$$

recalling that

$$\varepsilon_W = \frac{W^2 - 2m^2}{2W} \tag{2-18}$$

$$m_W = \frac{m^2}{W} \tag{2-19}$$

for this truncated Coulomb potential energy

$$V(r) = \frac{-\alpha}{r} \qquad (r > r_0) \tag{1-3}$$

$$V(r) = \frac{-\alpha}{r_0} \qquad (r < r_0) \tag{1-4}$$

First, the substitution of the constant potential energy of Eq. (1-4) into Eq. (2-21), leads to the differential equation

$$\frac{d^2u}{dr^2} + \tilde{K}^2 u(r) = 0 \tag{3-1}$$

where $\tilde{K}$ is a constant now defined as

$$\tilde{K} = \left[m_W^2 - \left(\varepsilon_W + \frac{\alpha}{r_0} \right)^2 \right]^{1/2} \tag{3-2}$$

Equation (3-1) is a well known equation, and its general solution is written immediately as

$$u(r) = c_1 \cos \tilde{K}r + c_2 \sin \tilde{K}r \tag{3-3}$$

where c_1 and c_2 are arbitrary constants. In order to have $u(r)/r$ remain finite at the origin, the constant c_1 is chosen as zero. Therefore, the physical solution to Eq. (3-1) is

$$u_I(r) = c_2 \sin \tilde{K}r \tag{3-4}$$

where the subscript I denotes Region I which is defined as the region in which $r < r_0$.

Next, we turn to Region II, or that region in which $r > r_0$. Substitution of the Coulomb potential Eq. (1-3)

$$V(r) = \frac{-\alpha}{r} \qquad (r > r_0) \tag{1-3}$$

into Eq. (2-21) leads to

$$\frac{d^2u}{dr^2} + \left[\varepsilon_W^2 - m_W^2 + \frac{2\varepsilon_W \alpha}{r} + \frac{\alpha^2}{r^2} \right] u(r) = 0 \tag{3-5}$$

Equation (3-5) is solved by transforming it into an equation with solutions that are recognized. (As a second method of obtaining and verifying the general solution asserted

here, Frobenius' method will be used to solve this differential equation in Chapter 4.) To proceed with the transformation, a change of variables is made such that

$$\rho = 2Kr \tag{3-6}$$

where

$$K = \left(m_W^2 - \varepsilon_W^2\right)^{1/2} \tag{3-7}$$

In continuing to make a change in variables, the chain rule of differentiation is used to derive the following relationship

$$\frac{d^2}{dr^2} = 4K^2 \frac{d^2}{d\rho^2} \tag{3-8}$$

Substitutions are made using Eqs. (3-8) and (3-6), leading to the transformation of Eq. (3-5) into the equation

$$\frac{d^2u}{d\rho^2} + \left[\frac{-1}{4} + \frac{k}{\rho} + \frac{\frac{1}{4} - \mu^2}{\rho^2}\right] u(\rho) = 0 \tag{3-9}$$

where

$$k = \frac{\varepsilon_W \alpha}{\left(m_W^2 - \varepsilon_W^2\right)^{1/2}} \tag{3-10}$$

$$\frac{1}{4} - \mu^2 = \alpha^2 \tag{3-11}$$

Equation (3-9) is Whittaker's equation, with solutions that are Whittaker functions (Arfken, 1985, p756). In mathematical terms, the general solution of Eq. (3-9) is

$$u(\rho) = c_3 M_{k,\mu}(\rho) + c_4 W_{k,\mu}(\rho) \tag{3-12}$$

where c_3 and c_4 are arbitrary constants, and

$$M_{k,\mu}(\rho) = e^{-\rho/2} \rho^{\frac{1}{2}+\mu} \, {}_1F_1\left(\tfrac{1}{2} + \mu - k, 1 + 2\mu; \rho\right) \tag{3-13a}$$

where

$$ {}_1F_1(a,c;x) = 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)}\frac{x^2}{2!} + \cdots, \qquad c \neq 0,-1,-2,\ldots \tag{3-13b} $$

and

$$ W_{k,\mu}(\rho) = e^{-\rho/2}\rho^{\frac{1}{2}+\mu}\, U\left(\tfrac{1}{2}+\mu-k, 1+2\mu; \rho\right) \tag{3-14a} $$

where

$$ U(a,c;x) = \frac{\pi}{\sin \pi c}\left[\frac{{}_1F_1(a,c;x)}{(a-c)!(c-1)!} - \frac{x^{1-c}\,{}_1F_1(a+1-c, 2-c; x)}{(a-1)!(1-c)!}\right] \tag{3-14b} $$

(Arfken, 1985, p. 753). The asymptotic expansions of Eqs. (3-13b) and (3-14b) are also found in Arfken (1985, p. 757), and are, respectively

$$ \frac{\Gamma(c)}{\Gamma(a)}\frac{e^x}{x^{c-a}}\left\{1 + \frac{(1-a)(c-a)}{1!x} + \frac{(1-a)(2-a)(c-a)(c-a+1)}{2!x^2} + \cdots\right\} \tag{3-15} $$

$$ \frac{1}{x^a}\left\{1 + \frac{a(1+a-c)}{1!(-x)} + \frac{a(a+1)(1+a-c)(2+a-c)}{2!(-x)^2} + \cdots\right\} \tag{3-16} $$

From Eq. (3-15), we see that the exponential term of this expansion dominates as $x \to \infty$. Therefore, in order to have $u(r)/r$ remain finite at infinity, we pick $c_3 = 0$, and conclude that the physical solution to Eq. (3-9) in Region *II* is

$$ u_{II}(\rho) = c_4 W_{k,\mu}(\rho) \tag{3-17} $$

Having obtained the solutions to Eq. (2-21) in Regions *I* and *II*, the boundary conditions on these solutions are now applied, which are that the two solutions and their first derivatives match at $r = r_0$. Another way of describing this step is to say that the logarithmic derivatives of the two solutions need to match at $r = r_0$. Stated mathematically, we have

$$ c_2 \sin \tilde{K} r_0 = c_4 W_{k,\mu}(\rho)\Big|_{r=r_0} \tag{3-18} $$

and

$$ \tilde{K} c_2 \cos \tilde{K} r_0 = (d/dr) c_4 W_{k,\mu}(\rho)\Big|_{r=r_0} \tag{3-19} $$

Dividing Eq. (3-19) by Eq. (3-18) gives

$$\tilde{K}\cot\tilde{K}r_0 = \left.\frac{(d/dr)W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)}\right|_{r=r_0} \tag{3-20}$$

Equation (3-20) is a transcendental equation in $W/2m$, the center-of-mass energy of SCP divided by the mass of the electron plus the positron. Solving Eq. (3-20) for $W/2m$ as a function of α is the work of the next sections.

3-2 Choosing the degrees of freedom. In this section, algebraic steps are taken in order to write Eq. (3-20)

$$\tilde{K}\cot\tilde{K}r_0 = \left.\frac{(d/dr)W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)}\right|_{r=r_0} \tag{3-20}$$

as an equation of the three variables $W/2m$, α, and mr_0, where W is the energy of SCP in the center-of-mass frame, m is the mass of the electron, r_0 is an arbitrarily small cut-off radius, and α is the coupling constant. This task is equivalent to writing $\tilde{K}$, k, μ, and ρ in terms of $W/2m$, α, and mr_0.

To begin with, μ is straightforward as it depends only on α. Rearranging Eq. (3-11) we find that

$$\mu = \left(\tfrac{1}{4} - \alpha^2\right) \tag{3-21}$$

Next, consider $\rho = 2Kr$, where

$$K = \left(m_W^2 - \varepsilon_W^2\right)^{1/2} \tag{3-7}$$

$$\varepsilon_W = \frac{W^2 - 2m^2}{2W} \tag{3-3}$$

$$m_W = \frac{m^2}{W} \tag{3-4}$$

Multiplying and dividing Eq. (3-3) by $4m^2$, leads to

$$\varepsilon_W = m\left[\frac{y^2 - \frac{1}{2}}{y}\right] \tag{3-22}$$

where y is defined as $y = W/2m$. From Eq. (3-4), we see that $m_W = m/2y$. Furthermore, by substituting this last expression and Eq. (3-22) back into Eq. (3-7), we find that

$$K = \pm m\left[\left(\frac{1}{2y}\right)^2 - \left(\frac{y^2 - \frac{1}{2}}{y}\right)^2\right]^{\frac{1}{2}} \tag{3-23}$$

Expanding, simplifying, and keeping the positive root in Eq. (3-23), K becomes

$$K = \left(m_W^2 - \varepsilon_W^2\right)^{\frac{1}{2}} = m\left(1 - y^2\right)^{\frac{1}{2}} \tag{3-24}$$

Therefore, with the help of Eq. (3-24), it follows that

$$\rho = 2Kr = 2\left(1 - y^2\right)^{1/2} mr \tag{3-25}$$

an equation expressing ρ in terms of y, and mr_0 when r is evaluated at r_0.

Consider next k, one of the indices of the Whittaker function:

$$k = \frac{\varepsilon_W \alpha}{\left(m_W^2 - \varepsilon_W^2\right)^{\frac{1}{2}}} \tag{3-10}$$

Using Eqs. (3-22) and (3-24), we find that

$$k = \frac{\left(y^2 - \frac{1}{2}\right)\alpha}{y\left(1 - y^2\right)^{1/2}} \tag{3-26}$$

Finally, we obtain the corresponding expression of $\tilde{K}$:

$$\tilde{K} = \left[m_W^2 - \left(\varepsilon_W + \frac{\alpha}{r_0} \right)^2 \right]^{1/2} \tag{3-2}$$

Using Eq. (3-22) in order to make a substitution for ε_W, and with $m_W = m/2y$, Eq. (3-2) in terms of y, mr_0, and α, becomes

$$\tilde{K} = m\left[\left(1 - y^2\right) - \frac{2\left(y^2 - \tfrac{1}{2}\right)\alpha}{ymr_0} - \left(\frac{\alpha}{mr_0} \right)^2 \right]^{1/2} \tag{3-27}$$

The lone factor of m in Eq. (3-27) does indeed match up with a factor of r_0 in the transcendental equation, Eq. (3-20), as, by inspection, there is an r_0 that multiplies $\tilde{K}$ inside the argument of the cotangent, and, as will be seen later, there is an r_0 that will come from the right hand side of Eq. (3-20) to combine with the $\tilde{K}$ which is outside of the cotangent.

In summary, the $\tilde{K}$, k, μ, and ρ, of Eq. (3-20), and therefore Eq. (3-20) itself, have all been written in terms of $W/2m$, α, and mr_0. We now choose to solve Eq. (3-20) for $W/2m$ by fixing mr_0 and allowing α to vary. The end result will be graphs of $W/2m$ versus α, with each curve being labeled for a given mr_0. In order to solve Eq. (3-20) using the software *Mathematica*, however, it will first be necessary to perform a few more algebraic calculations.

3-3 The secant method and *Mathematica*. The following recursion formula (Abramowitz, 1972, p. 507) is an important formula in solving Eq. (3-20) with *Mathematica*:

$$\rho W'_{k,\mu}(\rho) = \left(\tfrac{1}{2}\rho - k\right) W_{k,\mu}(\rho) - W_{k+1,\mu}(\rho) \tag{3-28}$$

The prime in this equation means the derivative with respect to ρ. The importance of this recursion formula is that it can be used to express the right hand side of Eq. (3-20) in terms of unprimed Whittaker functions. Implementation of Eq. (3-28) begins by dividing it through by $\rho W_{k,\mu}(\rho)$ to obtain

$$\frac{W'_{k,\mu}(\rho)}{W_{k,\mu}(\rho)} = \frac{1}{\rho}\left[\left(\tfrac{1}{2}\rho - k\right) - \frac{W_{k+1,\mu}(\rho)}{W_{k,\mu}(\rho)}\right] \tag{3-29}$$

Using the chain rule and recalling that $\rho = 2Kr$, we find that $(d/d\rho) = (1/2K)(d/dr)$, which leads to the expression of Eq. (3-29) as

$$\frac{(d/dr)W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)} = \frac{1}{r}\left[\left(\tfrac{1}{2}\rho - k\right) - \frac{W_{k+1,\mu}(\rho)}{W_{k,\mu}(\rho)}\right] \tag{3-30}$$

This expression is exactly the right-hand side of Eq. (3-20) in terms of unprimed Whittaker functions.

Since it is the confluent hypergeometric function $U(a,c;x)$ of the Whittaker function, (see Eqs. (3-14a) and (3-14b)) that is built into *Mathematica*, Eq. (3-30) in its most useful form is

$$\frac{(d/dr)W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)} = \frac{1}{r}\left[\left(\tfrac{1}{2}\rho - k\right) - \frac{U(\mu - k - \tfrac{1}{2}, 2\mu + 1; \rho)}{U(\mu - k + \tfrac{1}{2}, 2\mu + 1; \rho)}\right] \tag{3-31}$$

Note that after evaluation at $r = r_0$, it is the $1/r$ term of Eq. (3-31) that combines with the lone factor of m in Eq. (3-27) leading to an mr_0, as discussed at the end of the previous section.

Equation (3-31), evaluated at $r = r_0$, and $\tilde{K}\cot\tilde{K}r_0$ are now written in terms of $W/2m$, α, and mr_0, by using Eqs. (3-27), (3-26), (3-21), and (3-25) to make substitutions for $\tilde{K}$, k, μ, and ρ, respectively. We find that the bracketed quantity in Eq. (3-31), in terms of $W/2m$, α, and mr_0, is

$$\left[M\left(1-y^2\right)^{1/2} - \frac{\alpha\left(y^2 - \tfrac{1}{2}\right)}{y\left(1-y^2\right)^{1/2}} - \frac{U\left(\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} - \dfrac{\alpha\left(y^2-\tfrac{1}{2}\right)}{y\left(1-y^2\right)^{1/2}} - \dfrac{1}{2}, 2\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} + 1, 2M\left(1-y^2\right)^{1/2}\right)}{U\left(\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} - \dfrac{\alpha\left(y^2-\tfrac{1}{2}\right)}{y\left(1-y^2\right)^{1/2}} + \dfrac{1}{2}, 2\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} + 1, 2M\left(1-y^2\right)^{1/2}\right)}\right] \tag{3-32}$$

where, for convenience in working with *Mathematica*, we have defined $M = mr_0$ and $y = W/2m$. (Furthermore, the symbol α would have to be replaced by a symbol such as

a, as *Mathematica* lacks Greek symbols.) This equation is Eq. (3-32) and will also be referred to as f.

Similarly, the left hand side of Eq. (3-20), $\tilde{K}\cot\tilde{K}r_0$, multiplied by r_0, is

$$g = M\left[\left(1-y^2\right)-\frac{2\alpha\left(y^2-½\right)}{yM}-\frac{\alpha^2}{M^2}\right]^{½}\cot\left\{M\left[\left(1-y^2\right)-\frac{2\alpha\left(y^2-½\right)}{yM}-\frac{\alpha^2}{M^2}\right]^{½}\right\} \tag{3-33}$$

The above equation is Eq. (3-33) and shall also be referred to as g.

The equations f and g are functions of the variables (α, y, M). We now choose to fix α and M, and find y such that $g(y)=f(y)$. The secant method, built into the software package *Mathematica*, is used to find numerical values for y. *Mathematica* can also run a Newton's method program. A review of Newton's method and the secant method, and the commands to implement them on *Mathematica* is briefly presented here.

In the equation $g(y)=f(y)$, an $F(y)$ can be defined as

$$F(y)=f(y)-g(y)=0 \tag{3-34}$$

In a Taylor series expansion, the first two terms approximate $F(y)$ as

$$F(y)\approx F(y_0)+(y-y_0)F'(y_0) \tag{3-35}$$

Since $F(y)$=0, Eq. (3-35) can be rearranged as

$$y\approx y_0-\frac{F(y_0)}{F'(y_0)} \tag{3-36}$$

Given an initial "root" as y_0, Eq. (3-36) is used to compute y, which in turn becomes the next y_0, beginning a loop of calculations. *Mathematica* ends the loop when a specified accuracy is reached. The command that is given to Mathematica to run Newton's method is

$$\text{FindRoot}[lhs == rhs, \{y, y_0\}] \tag{3-37}$$

where the initial "root" goes in the y_0 slot, f in the *lhs* slot, and g in the *rhs* slot. The downfall of Newton's method in this case, referring back to the expressions for f and g,

is that the first derivative of $F(y)$ *with respect to* y is required. Since *Mathematica* could not compute the required derivative symbolically, we turn to the secant method.

The secant method, of course, circumvents the necessity of having the first derivative as required by Newton's Method. To see this, the approximation

$$F'(y_0) \approx \frac{F(y_1) - F(y_0)}{y_1 - y_0} \tag{3-38}$$

is assumed, and substituted back into Eq. (3-36), leading to

$$y = y_0 - \frac{F(y_0)(y_1 - y_0)}{F(y_1) - F(y_0)} \tag{3-39}$$

The command given to *Mathematica* to run the secant method is

$$\text{FindRoot}\left[lhs == rhs, \{y, \{y_0, y_1\}\}\right] \tag{3-40}$$

Two initial "roots" are required here, but once provided in the y_0 and y_1 slots and initiating the secant method, *Mathematica* successfully returns y, for a fixed α and mr_0. (One way of obtaining numerical values for y_0 and y_1 in Eq. (3-38) is to have *Mathematica* plot f and g on the same graph and then read off two labeled points from the horizontal axis that are close to the actual root.) The data is given in Tables 3-1 to 3-6 and curves of $W/2m$ versus α for fixed values of mr_0 are plotted in Fig (3-1), all of which are compiled at the conclusion of this chapter.

3-4 A prediction of stability. In Fig. (3-1), a vertical line is drawn at $\alpha = 1/2$, dividing the graph into two regions for discussion. This line is significant because we may not expect to see stability or instability only until after crossing this line in the direction of increasing α. This expectation is based upon the problem of a Klein-Gordon particle in a strong Coulomb field (Fried 1991, p. 52), from which Fig. (3-2) is taken. Specifically, the Klein-Gordon equation, using the same interaction of Eqs. (1-3) and (1-4), but where α is replaced by $Z\alpha$, and with α reassuming its physical value, describing a pion in the strong field of a heavy ion of variable charge Z, predicts that just after $Z = 68$ there is a Z beyond which the energy of the pion dives below $-m$.

Therefore, based upon the result summarized in Fig. (3-2), we may be biased in our two-particle, equal mass problem, to find an α beyond $\alpha = 1/2$, such that $W/2m$ dives below 0. Inspection of Fig. (3-1) in the region of $\alpha > 1/2$, however, shows that there is no such α, and that the Crater and Van Alstine equation of Eq. (2-21) stands in sharp contrast with the result of instability obtained from the Klein-Gordon equation in the problem described above. Furthermore, as mentioned in Chapter 2 and referring to Fig. (2-1), "these results are in sharp contrast with corresponding results from the Dirac equation, even though the CV equations correctly reduce to the Dirac equation when the mass of one of the particles becomes infinite. Thus, the stability properties of a two-body system with equal masses may be quite different from the unequal mass case, at least if one trusts the CV equations in the nonperturbative regime" (Bawin, 1990), where CV denotes Crater and Van Alstine.

In the region of $\alpha < 1/2$ of Fig. (3-1), data points are noticeably missing, with the exception of points at $\alpha = 65/137$. *Mathematica* did return other values of $W/2m$ in this region, but as α decreased, the program indicated that such roots were not within the prescribed accuracy after its default number of fifteen iterations. One way to avoid this flag was to give *Mathematica* two new initial guesses that were in close agreement out to several decimal places with the root that was returned with the flag. The expected behavior of the roots in this region, however, have ultimately been estimated here with a dotted line in Fig. (3-1), using end points of $W/2m = 1$, for the free particle with $\alpha = 0$, and the root that was reported for a bound state at $\alpha = 65/137$. Diving below zero is not expected in this region.

Our main result of this chapter is the derivation of Fig. (3-1), which recovers an earlier plot of $W/2m$ versus α for fixed values of mr_0 (Bawin 1990). We will now change the truncating potential to see if such a change makes a difference in the prediction of stability that was found here.

TABLE 3-1

$mr_0 = 0.005$

α	$W/2m$
65/137	0.955227
70/137	0.940571
75/137	0.91832
80/137	0.882261
85/137	0.822378
90/137	0.729538
95/137	0.601955
100/137	0.463908
105/137	0.342978
110/137	0.252598
115/137	0.189766
120/137	0.146569
125/137	0.116359
130/137	0.0946685
135/137	0.0786647
140/137	0.0665525
145/137	0.0571745
150/137	0.0497665
155/137	0.0438103
160/137	0.0389464
165/137	0.0349196
170/137	0.0315451
175/137	0.0286863
180/137	0.0262409

TABLE 3-2

$mr_0 = 0.001$

α	$W/2m$
65/137	0.953764
70/137	0.936056
75/137	0.903075
80/137	0.828607
85/137	0.660836
90/137	0.41309
95/137	0.224924
100/137	0.128718
105/137	0.0808856
110/137	0.055022
115/137	0.0397794
120/137	0.0301354
125/137	0.0236771
130/137	0.01915
135/137	0.0158562
140/137	0.0133847
145/137	0.0114818
150/137	0.0099841
155/137	0.008783
160/137	0.00780394

TABLE 3-3

$mr_0 = 0.0001$

α	$W/2m$
65/137	0.952635
70/137	0.930682
72/137	0.914596
74/137	0.887845
75/137	0.867018
77/137	0.796947
78/137	0.739966
80/137	0.570407
81/137	0.466949
82/137	0.3667
83/137	0.280924
85/137	0.163879
87/137	0.100334
90/137	0.0538241
91/137	0.0449076
92/137	0.037894
93/137	0.032305
94/137	0.0277974
95/137	0.0241217
100/137	0.01316
105/137	0.00816
110/137	0.00552

TABLE 3-4

$mr_0 = 0.00001$

α	$W/2m$
65/137	0.952092
70/137	0.92591
72/137	0.900132
74/137	0.834452
75/137	0.759611
76/137	0.631225
77/137	0.453345
78/137	0.283515
79/137	0.169449
80/137	0.103965
81/137	0.066808
82/137	0.0449294
83/137	0.0314496
84/137	0.0227828
85/137	0.0169964
86/137	0.0130038
87/137	0.010169
90/137	0.00540308

TABLE 3-5

$mr_0 = 0.000001$

α	$W/2m$
65/137	0.951831
70/137	0.921203
71/137	0.905084
72/137	0.874512
73/137	0.803581
74/137	0.626785
75/137	0.336896
76/137	0.141734
77/137	0.0633911
78/137	0.0318247
79/137	0.0176212
80/137	0.0105478
81/137	0.00672048

TABLE 3-6

$mr_0 = 0.0000001$

α	$W/2m$
65/137	0.951705
70/137	0.916038
71/137	0.888679
72/137	0.804709
73/137	0.495539
74/137	0.138974
75/137	0.039898
76/137	0.0145635
77/137	0.006373
78/137	0.00318674
79/137	0.00176284
80/137	0.00105493

FIG. 3-1. Center-of-momentum energy versus field strength for a constant truncation of the Coulomb potential (Crater and Van Alstine equation).

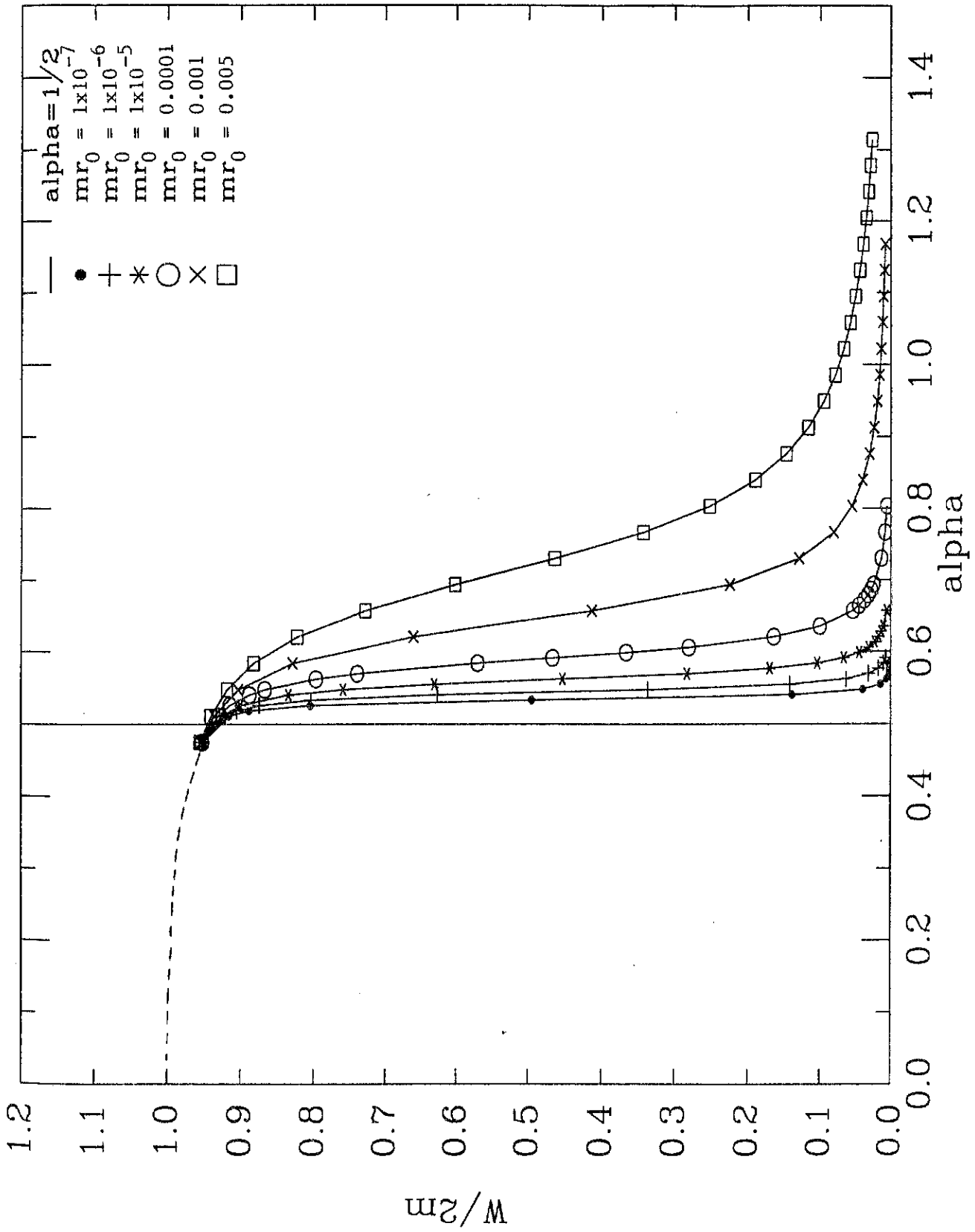


FIG. 3-2. Instability of the Klein-Gordon equation in a strong field for a constant truncation of the Coulomb potential (Fried, 1991, p. 53).

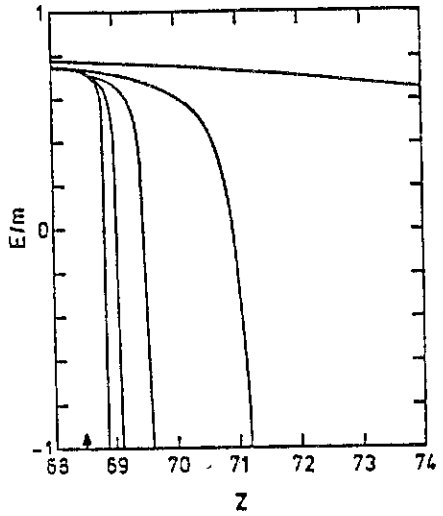


Fig. 1. 1s bound-state energy spectrum for a Klein-Gordon particle with interaction (1)-(2) as a function of the external charge Z. The different curves (from upper right to lower left) refer to a radius $r_0 = 10^{-3}, 10^{-9}, 10^{-15}, 10^{-21}$ and 10^{-27} fm, respectively, and to m = pion mass. Note that our results hold for any mass, provided that the radius r_0 is rescaled in such a way that mr_0 keeps a constant value.

CHAPTER 4

A QUADRATIC TRUNCATING POTENTIAL

Strongly coupled positronium in the ${}^1S_0$ state is being described by a differential equation that is formally identical to the S-wave radial Klein-Gordon equation. This differential equation is presently solved again for the Coulomb potential, but in this chapter, a quadratic truncating potential is used in place of the truncating constant potential of Chapter 3. A transcendental equation, resulting from matching the logarithmic derivatives of the two solutions, will be solved to find the center-of-momentum energy of strongly coupled positronium as a function of α, the fine structure constant, leading to a prediction of stability or instability with regard to spontaneous, real, electron positron pair creation.

4-1 Frobenius' method and the Coulomb potential. Equation (2-21), formally identical to the S-wave radial Klein-Gordon equation,

$$\frac{d^2u}{dr^2}+\left[\left(\varepsilon_W-V\right)^2-m_W^2\right]u(r)=0 \tag{2-21}$$

is used here to describe the ${}^1S_0$ state of strongly coupled positronium. In this chapter, Eq. (2-21) will be studied for the following potential:

$$V(r)=\frac{-\alpha}{r} \qquad (r>r_0) \tag{1-3}$$

$$V(r)=\frac{3\alpha}{2r_0^3}\left[\frac{r^2}{3}-r_0^2\right] \qquad (r<r_0) \tag{1-5}$$

where r_0 is an arbitrarily small cut-off radius, and α is the coupling constant.

The substitution of Eq. (1-3) first into Eq. (2-21), leads to

$$\frac{d^2u}{dr^2}+\left[\varepsilon_W^2-m_W^2+\frac{2\varepsilon_W\alpha}{r}+\frac{\alpha^2}{r^2}\right]u(r)=0 \tag{3-5}$$

In Chapter 3, Eq. (3-5) was solved by transforming it into Whittaker's equation, the two solutions to which are, of course, Whittaker functions. For the purpose of demonstration and to confirm that Whittaker functions are indeed the solutions, Eq. (3-5) is solved here using Frobenius' method

To begin, Eq. (3-5) is examined in the limit $r \to \infty$. In this limit, Eq. (3-5) becomes

$$u'' - K^2 u = 0 \qquad r \to \infty \tag{4-1}$$

where

$$K^2 = m_W^2 - \varepsilon_W^2 \tag{4-2}$$

(The above definition of K^2 is made to be in agreement with Eq. (3-7), in anticipation of the comparison of the solution of Chapter 3 with the solution obtained presently.) Of the two solutions to Eq. (4-1), the one that does not blow up at $r \to \infty$ is $\exp(-Kr)$; therefore, $u(r)$ is now assumed to be of the form

$$u(r) = \exp(-Kr) f(r) \tag{4-3}$$

where

$$f(r) = \sum_{n=0}^{\infty} a_n r^{n+\lambda} \qquad a_0 \neq 0 \tag{4-4}$$

Having extracted the asymptotic behavior of $u(r)$, Eq. (4-3) is substituted back into Eq. (3-5), leading to the following differential equation for $f(r)$:

$$f'' - 2Kf' + \left(\frac{\alpha^2}{r^2} + \frac{2\varepsilon_W \alpha}{r} \right) f = 0 \tag{4-5}$$

or

$$\sum_{n=0}^{\infty} \left[(n+\lambda)(n+\lambda-1) + \alpha^2 \right] a_n r^{n+\lambda-2} + \sum_{n=0}^{\infty} \left[2\varepsilon_W \alpha - 2K(n+\lambda) \right] a_n r^{n+\lambda-1} = 0 \tag{4-6}$$

Equation (4-6) is satisfied by solving individual equations the terms of which are all of the same power in r. The lowest order term in Eq. (4-6) is the $r^{\lambda-2}$ term, and since there is only one of these terms, we find that

$$\left(\lambda^2 - \lambda + \alpha^2 \right) a_0 r^{\lambda-2} = 0 \tag{4-7}$$

In Eq. (4-7), since $a_0 \neq 0$, the quadratic equation in the brackets, known as the indicial equation, must be equal to zero. Using the quadratic formula, the index λ is determined to be either one of the following values:

$$\lambda = \frac{1}{2} \pm \mu \tag{4-8}$$

where

$$\mu = \sqrt{\tfrac{1}{4} - \alpha^2} \tag{4-9}$$

The above definition of μ is made intentionally to match Eq. (3-13).

The remaining higher order equations, contained in Eq. (4-6), that are in like power of r, can be satisfied, in this case, in general. A general equation describing terms of order $m + \lambda - 1$ is the following:

$$\left[(m+\lambda)(m+\lambda+1)+\alpha^2\right]a_{m+1}r^{m+\lambda-1} + \left[2\varepsilon_W\alpha - 2K(m+\lambda)\right]a_m r^{m+\lambda-1} = 0 \tag{4-10}$$

Equation (4-10) is satisfied if

$$a_{m+1} = \frac{2K\left[(m+\lambda)-k\right]a_m}{\left[(m+\lambda)(m+\lambda+1)+\alpha^2\right]} \tag{4-11}$$

where

$$k = \frac{\varepsilon_W\alpha}{\left(m_W^2 - \varepsilon_W^2\right)^{1/2}} \tag{4-12}$$

The definition of Eq. (4-12) is made to be in agreement with Eq. (3-10). Equation (4-11) is a recursion relationship between coefficients in the power series solution, Eq. (4-4). We now proceed by writing out the terms of $u(r)$ for each of the specific values of λ.

The positive root, $\lambda = (1/2) + \mu$, is considered first and in addition to $\alpha^2 = (1/4) - \mu^2$ from Eq. (4-9), substitutions are made into Eq. (4-11), leading to

$$a_{m+1} = \frac{a_m\left(m+\mu-k+\frac{1}{2}\right)2K}{(m+1+2\mu)(m+1)} \tag{4-13}$$

We use this recursion relationship and substitute Eq. (4-4) into Eq. (4-3) in order to rewrite $u(r)$ more compactly as

$$u(r) = e^{-Kr} r^{\lambda} \sum_{n=0}^{\infty} a_n r^n \tag{4-14}$$

We find that the first few terms of $u(r)$, in the case of $\lambda = (1/2) + \mu$, are

$$u(r) = c_1 e^{\frac{-\rho}{2}} \rho^{\frac{1}{2}+\mu} \left\{ 1 + \frac{(\mu - k + \frac{1}{2})}{(1+2\mu)} \frac{\rho}{1!} + \frac{(\mu - k + \frac{1}{2})(\mu - k + \frac{3}{2})}{(1+2\mu)(2+2\mu)} \frac{\rho^2}{2!} + \cdots \right\} \tag{4-15}$$

where $\rho = 2Kr$ and the arbitrary constant a_0 has been defined as $a_0 = c_1 (2K)^{\frac{1}{2}+\mu}$. The infinite series in the brackets of Eq. (4-15) is identified as the confluent hypergeometric function, ${}_1F_1(\mu - k + \frac{1}{2}, 1 + 2\mu; \rho)$, first encountered in Eq. (3-13b). Therefore, suppressing momentarily the arbitrary constant c_1, we see that Eq. (4-15) is exactly the Whittaker function, $M_{k,\mu}(\rho)$, of Eq. (3-13a).

We now recover the second Whittaker function. Switching from the positive root to $\lambda = (1/2) - \mu$, the negative root in Eq. (4-8), we find that the algebra outlined in the paragraph above leads to analogous relationships with the only difference being that $-\mu$ ultimately replaces μ everywhere in Eq. (4-15). Therefore, the Frobenius' method yields $M_{k,-\mu}(\rho)$ as our second solution to Eq. (3-5).

Since it is the Whittaker function $W_{k,\mu}(\rho)$, first encountered in Eq. (3-14a), that is preferred over $M_{k,-\mu}(\rho)$ as the second solution to Eq. (3-5), the following linear combination of $M_{k,\mu}(\rho)$ and $M_{k,-\mu}(\rho)$ is used to construct $W_{k,\mu}(\rho)$:

$$W_{k,\mu}(\rho) = \frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2} - \mu - k)} M_{k,\mu}(\rho) + \frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2} + \mu - k)} M_{k,-\mu}(\rho) \tag{4-16}$$

(Abramowitz, 1972, p. 505). Thus, we recover the second solution claimed in Chapter 3.

In Summary, the ${}^1S_0$ state of strongly coupled positronium can be described by Eq. (2-21). The Coulomb potential substituted into this equation leads to Eq. (3-5). In turn, solving Eq. (3-5), this time using Frobenius' method, confirms the general solution as

$$u(\rho) = c_1 M_{k,\mu}(\rho) + c_2 W_{k,\mu}(\rho) \tag{4-17}$$

Furthermore, in Chapter 3 and using Eq. (3-15), we have seen that the constant next to $M_{k,\mu}(\rho)$ should be set equal to zero in order to have $u(r)/r$ remain finite as $r \to \infty$.

Therefore, with $c_1 = 0$, we conclude that in the region in which $r > r_0$, or Region II, the solution to Eq. (2-21) is

$$u_{II}(\rho) = c_2 W_{k,\mu}(\rho) \tag{4-18}$$

A quadratic potential, given in Eq. (1-5), is to be used as a truncating potential of the Coulomb potential in the region $r < r_0$, or Region I, where r_0 is an arbitrarily small cut-off radius. The need for truncating the potential is to avoid the singularity of the Coulomb potential at $r = 0$ and to have access to α beyond 1/2. Equation (1-5) now replaces the potential $A(r) = -\alpha/r_0$ of Chapter 3 as the truncating potential for the purpose of determining whether this change affects the prediction of stability with regard to pair creation.

4-2 Frobenius' method and a quadratic potential. In this section, Eq. (2-21),

$$\frac{d^2u}{dr^2} + \left[(\varepsilon_W - V)^2 - m_W^2\right] u(r) = 0 \tag{2-21}$$

is solved with a quadratic potential, specifically

$$V(r) = \frac{3\alpha}{2r_0^3}\left[\frac{r^2}{3} - r_0^2\right] \qquad (r < r_0) \tag{1-5}$$

Substitution of Eq. (1-5) into Eq. (2-21), leads to

$$\left[\frac{d^2}{dr^2} + \delta r^4 + \gamma r^2 + \beta\right] u(r) = 0 \tag{4-19}$$

where

$$\delta = \frac{\alpha^2}{4r_0^6} \tag{4-20}$$

$$\gamma = -\left(\frac{3\alpha^2}{2r_0^4} + \frac{\varepsilon_W \alpha}{4r_0^3}\right) \tag{4-21}$$

$$\beta = -\left(m_W^2 - \varepsilon_W^2\right) + \frac{9\alpha^2}{4r_0^2} + \frac{3\varepsilon_W \alpha}{r_0} \tag{4-22}$$

Equation (4-19) is to be solved using Frobenius' method, and therefore, a power series solution, of the form

$$u(r) = \sum_{n=0}^{\infty} a_n r^{n+\lambda} \qquad a_0 \neq 0 \tag{4-23}$$

is assumed, and substituted back into the differential equation. After the substitution, Eq. (4-19) can be written as

$$r^{\lambda} \sum_{n=0}^{\infty} a_n \left[(n+\lambda)(n+\lambda-1) r^{n-2} + \delta r^{n+4} + \gamma r^{n+2} + \beta r^n \right] = 0 \tag{4-24}$$

Finding the lowest order term in r of Eq. (4-24), we see that the indicial equation is $\lambda(\lambda - 1) = 0$, such that $\lambda = 0$ and $\lambda = 1$. Handling all of the higher order terms by writing out a general equation, as done with the Coulomb potential, does not yield a two-term recursion relationship between coefficients. This fact makes the problem messy, algebraically speaking, in determining the coefficients because equations in the same power of r will have to be generated from Eq. (4-24) and analyzed individually, and not all at once in a two-term recursion relationship.

We select $\lambda = 0$ to analyze first. Terms of Eq. (4-24) are written out for $n = 1$ up to, say, 5. Then, terms of like power in r are collected to give the following five equalities:

$$r^0 \text{ terms:} \quad \beta a_0 + 2a_2 = 0 \tag{4-25}$$

$$r^1 \text{ terms:} \quad \beta a_1 + 3 \cdot 2 a_3 = 0 \tag{4-26}$$

$$r^2 \text{ terms:} \quad \gamma a_0 + \beta a_2 + 4 \cdot 3 a_4 = 0 \tag{4-27}$$

$$r^3 \text{ terms:} \quad \gamma a_1 + \beta a_3 + 5 \cdot 4 a_5 = 0 \tag{4-28}$$

From Eq. (4-25), we have

$$a_2 = \frac{-\beta}{2} a_0 \tag{4-29}$$

Substituting Eq. (4-29) into Eq. (4-27), leads to

$$a_4 = \frac{1}{4 \cdot 3}\left(\frac{\beta^2}{2} - \gamma\right) a_0 \tag{4-30}$$

Similarly, from Eq. (4-26), we have

$$a_3 = \frac{-\beta}{3 \cdot 2} a_1 \tag{4-31}$$

Substituting Eq. (4-31) into Eq. (4-28), leads to

$$a_5 = \frac{1}{5 \cdot 4}\left(\frac{\beta^2}{3 \cdot 2} - \gamma\right) a_1 \tag{4-32}$$

With coefficients a_0 up through a_5 in hand, Eq. (4-23) gives the solution of Eq. (4-19), corresponding to $\lambda = 0$, approximately as

$$u(r) = a_0\left[1 - \frac{\beta}{2} r^2 + \frac{1}{4 \cdot 3}\left(\frac{\beta^2}{2} - \gamma\right) r^4 + \cdots\right] + a_1\left[r - \frac{\beta}{3 \cdot 2} r^3 + \frac{1}{5 \cdot 4}\left(\frac{\beta^2}{3 \cdot 2} - \gamma\right) r^5 + \cdots\right] \tag{4-33}$$

Note that Eq. (4-33) is an even series plus an odd series, and in this way, it is reminiscent of the sine and cosine solutions associated with the truncating potential of Chapter 3.

It is redundant to analyze Eq. (4-24) with $\lambda = 1$ because the two acceptable values of λ differ by a positive integer, in this case, meaning that the smaller value, $\lambda = 0$, either yields two independent solutions or no solutions in the form of a power series (Hildebrand, 1976, p. 131). Thus, Eq. (4-33) is taken to be the general solution to Eq. (4-19). The physical solution is found by demanding that $u(r)/r$ remain finite at $r = 0$. Therefore, the constant a_0 is chosen as zero, and in Region I we have

$$u_I(r) = a_1\left[r - \frac{\beta}{3 \cdot 2} r^3 + \frac{1}{5 \cdot 4}\left(\frac{\beta^2}{3 \cdot 2} - \gamma\right) r^5 + \cdots\right] \tag{4-34}$$

where

$$\gamma = -\left(\frac{3\alpha^2}{2r_0^4} + \frac{\varepsilon_W \alpha}{4r_0^3}\right) \tag{4-21}$$

$$\beta = -\left(m_W^2 - \varepsilon_W^2\right) + \frac{9\alpha^2}{4r_0^2} + \frac{3\varepsilon_W \alpha}{r_0} \tag{4-22}$$

As a final note in working with Eq. (4-34), we must now decide how many terms to keep in the series. Because in Region I the variable r is arbitrarily small, and in the interest of simplicity, $u_I(r)$ will first be approximated by

$$u_I(r) = a_1 r \tag{4-35}$$

in the next section. The consequences of keeping the first two terms and the first three terms of Eq. (4-34), however, are also discussed in this chapter. Equation (4-35) will now be matched with $u_{II}(\rho) = c_2 W_{k,\mu}(\rho)$ at the boundary $r = r_0$.

4-3 Finding the energy. Having a solution for Eq. (2-21) in Regions I and II, the steps taken in Chapter 3 to determine $W/2m$ as a function α for fixed values $\mathrm{m}r_0$ are followed here.

The boundary conditions on the solutions in Regions I and II are that the two solutions and their first derivatives match at $r = r_0$. Applying these boundary conditions to the solutions, Eqs. (4-35) and (4-18), leads to the following two equalities:

$$a_1 r_0 = c_2 W_{k,\mu}(\rho)\Big|_{r=r_0} \tag{4-36}$$

and

$$a_1 = (d/dr) c_2 W_{k,\mu}(\rho)\Big|_{r=r_0} \tag{4-37}$$

Dividing Eq. (4-37) by Eq. (4-36) gives

$$\frac{1}{r_0} = \frac{(d/dr) W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)}\Bigg|_{r=r_0} \tag{4-38}$$

an equation analogous to the transcendental equation Eq. (3-20). Prior to solving Eq. (4-38) for $W/2m$ as a function of α with *Mathematica*, the results of Chapter 3 are needed here. First of all, Eq. (3-30)

$$\frac{(d/dr)W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)} = \frac{1}{r}\left[\left(\tfrac{1}{2}\rho - k\right) - \frac{W_{k+1,\mu}(\rho)}{W_{k,\mu}(\rho)}\right] \tag{3-30}$$

is used to write Eq. (4-38) as

$$1 = \left[\left(\tfrac{1}{2}\rho - k\right) - \frac{U(\mu - k - \tfrac{1}{2}, 2\mu + 1; \rho)}{U(\mu - k + \tfrac{1}{2}, 2\mu + 1; \rho)}\right] \tag{4-39}$$

Then, in order to express the right-hand side of Eq. (4-39) in terms of $y(= W/2m)$, α, and $M(= mr_0)$, the function defined as f in Eq. (3-32):

$$\left[M\left(1-y^2\right)^{1/2} - \frac{\alpha\left(y^2 - \tfrac{1}{2}\right)}{y\left(1-y^2\right)^{1/2}} - \frac{U\left(\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} - \frac{\alpha\left(y^2-\tfrac{1}{2}\right)}{y\left(1-y^2\right)^{1/2}} - \frac{1}{2}, 2\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} + 1, 2M\left(1-y^2\right)^{1/2}\right)}{U\left(\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} - \frac{\alpha\left(y^2-\tfrac{1}{2}\right)}{y\left(1-y^2\right)^{1/2}} + \frac{1}{2}, 2\left(\tfrac{1}{4}-\alpha^2\right)^{1/2} + 1, 2M\left(1-y^2\right)^{1/2}\right)}\right] \tag{3-32}$$

is recalled, such that Eq. (4-38) becomes $1 = f$. The variable y can now be found for a given value of α and M, using the secant method and the software *Mathematica*.

A computer file containing f is created, if one does not exist already from the research of Chapter 3, and the secant method is implemented, for a given value for α and M, with the command

$$\text{FindRoot}\left[1 == f, \left\{y, \left\{y_0, y_1\right\}\right\}\right] \tag{4-40}$$

where numerical values close to an expected root are put in the y_0 and y_1 slots. The results of using Eq. (4-40) are tabulated in Tables (4-1) to (4-6), which in turn are plotted in Fig. (4-1). In Fig. (4-1), we see that there are only positive values of $W/2m$ as a function of α, indicating the same result of stability that was found in Chapter 3. It is also noted, however, that the values derived here for $W/2m$ have decreased compared with Chapter 3.

This feature might have been expected since the truncation of the potential of Eq. (1-5) provides a deeper potential well in comparison with the truncation of Eq. (1-4).

4-4 Keeping two terms. Before we reach final conclusions, the next step in this work is to approximate $u_I(r)$ with two terms kept in the series, or

$$u_I(r) = a_1\left[r - \frac{\beta}{3\cdot 2}r^3\right] \tag{4-41}$$

The boundary conditions are again applied to u_I, now given in Eq. (4-41), and u_{II}, which continues to be $u_{II}(\rho) = c_2 W_{k,\mu}(\rho)$. In so doing, the steps just taken in deriving Eq. (4-38) are followed, leading to a new transcendental equation:

$$\frac{1-\frac{\beta}{2}r_0^2}{r_0 - \frac{\beta}{3\cdot 2}r_0^3} = \left.\frac{(d/dr)W_{k,\mu}(\rho)}{W_{k,\mu}(\rho)}\right|_{r=r_0} \tag{4-42}$$

In order to express the left-hand side of Eq. (4-42) in terms of y, α, and M, first recall that β was defined as

$$\beta = -\left(m_W^2 - \varepsilon_W^2\right) + \frac{9\alpha^2}{4r_0^2} + \frac{3\varepsilon_W\alpha}{r_0} \tag{4-22}$$

Two substitutions are made into Eq. (4-22) using Eqs. (3-22) and (3-24). After algebraic computations, we find that

$$\beta = m^2\left[-\left(1-y^2\right) + \frac{9\alpha^2}{4M^2} + \frac{3\alpha}{M}\left(\frac{y^2 - \tfrac{1}{2}}{y}\right)\right] \tag{4-43}$$

Upon evaluating the right-hand side of Eq. (4-42) at $r = r_0$, note in reference to Eq. (3-31) that there is an r_0 that will be brought over and multiplied with the numerator on the left-hand side of Eq. (4-42). Therefore, with the help of Eq. (4-43), the left-hand side of Eq. (4-42), multiplied by r_0, in terms of y, α, and M, is defined as the function h and written as

$$h = \frac{1 - \frac{1}{8}\left[4M^2\left(y^2-1\right) + 9\alpha^2 + 12M\alpha\left(\frac{y^2 - \frac{1}{2}}{y}\right)\right]}{1 - \frac{1}{24}\left[4M^2\left(y^2-1\right) + 9\alpha^2 + 12M\alpha\left(\frac{y^2 - \frac{1}{2}}{y}\right)\right]} \tag{4-44}$$

Finally, after defining h in the computer, and specifying an α and an M, the command used in *Mathematica* to find $y = W/2m$, is

$$\text{FindRoot}\left[f == h, \left\{y, \left\{y_0, y_1\right\}\right\}\right] \tag{4-45}$$

The results of using Eq. (4-45) are found in Tables (4-7) to (4-12) and plotted in Fig. (4-2). From Fig. (4-2), we note that keeping two terms of the solution in Eq. (4-34) does not lead to a change in the result that only positive values of $W/2m$ as a function of α are found, but the data does show a faster drop-off of $W/2m$ for $\alpha > 1/2$ compared with Fig. (4-1). This faster dropping off led to keeping three terms in Eq. (4-34), the results of which are summarized in Tables (4-13) to (4-18) and plotted in Fig. (4-3). We observe that the curves of Fig. (4-3) are intermediate with respect to the curves of Fig. (4-1) and Fig. (4-2). This would suggest that convergence is taking place, such that keeping more and more terms would only lead to curves that are also intermediate with the extremes of Figs. (4-1) and (4-2). In conclusion, then, the main result is that Eq. (2-21) has been consistent, at least for the two choices of potentials in Chapters 3 and 4, in predicting stability with regard to spontaneous pair creation.

After completing the research of this thesis, it has come to our attention, that Greiner (1990, pp. 43-44), from which Fig. (4-4) is taken, has studied a pionic atom with the Klein-Gordon equation, using the potential of Eq. (1-3) and (1-5) to describe the interaction between the pion and a heavy nucleus. Greiner's study, in comparison with a study by Bawin in Fried (1991, p. 52), from which our Fig. 3-2 is taken, where the Klein-Gordon equation and the Coulomb potential with the truncation of Eq. (1-4) was used, is in agreement with the prediction of instability. Therefore, the Klein-Gordon equation is seen to be consistent with its prediction of stability for the unequal mass case, using either truncation of Eq. (1-3) or Eq. (1-4), whereas the Crater and Van Alstine equations represented by Eq. (2-21), has also been consistent with its prediction of stability in the equal mass case, for these two truncations.

At this point, we abruptly shift from our study of strongly coupled positronium using Eq. (2-21) to the subject of finding exactly solvable potentials--particularly potentials in the radial Klein-Gordon equation due to its relationship with Eq. (2-21)--using a method called matching of the constants. This change of subjects was made in an effort to find a closed form solution of the differential equation of Eq. (4-19), or even to derive another potential that has closed form solutions, and then to use it in place of the quadratic truncating potential. In hindsight, the solution of Eq. (4-19), found using Frobenius' method (Eq. (4-34)), was probably not as objectionable as it first appeared to be for use in this work. Nonetheless, the method of matching of the constants proved to be educational, applicable to strongly coupled positronium by way of Eq. (2-21), and important in its own right.

TABLE 4-1

$mr_0 = 0.005$

α	$W/2m$
55/137	0.973229
60/137	0.965445
65/137	0.954912
70/137	0.939718
75/137	0.915919
80/137	0.875511
85/137	0.804942
90/137	0.691486
95/137	0.542559
100/137	0.393755
105/137	0.277687
110/137	0.198892
115/137	0.147279
120/137	0.112935
125/137	0.0893352
130/137	0.0725563
135/137	0.060246
140/137	0.0509608
145/137	0.0437867
150/137	0.0381269
155/137	0.0335802
160/137	0.0298693
165/137	0.0267982

TABLE 4-2

$mr_0 = 0.001$

α	$W/2m$
60/137	0.964997
65/137	0.953577
70/137	0.935345
75/137	0.899908
80/137	0.813717
85/137	0.611653
90/137	0.343213
95/137	0.175462
100/137	0.098596
105/137	0.0616612
110/137	0.0418975
115/137	0.0302914
120/137	0.0229578
125/137	0.0180488
130/137	0.014608
135/137	0.0121043
140/137	0.0102253

TABLE 4-3

$mr_0 = 0.0001$

α	$W/2m$
60/137	0.964739
65/137	0.952545
70/137	0.930078
72/137	0.9131
74/137	0.88375
75/137	0.860039
77/137	0.776817
78/137	0.707623
80/137	0.508044
81/137	0.396945
82/137	0.298961
83/137	0.222253
85/137	0.125935
87/137	0.0763954
90/137	0.0408381
91/137	0.0340622
92/137	0.0287382
93/137	0.0244986
94/137	0.021081
95/137	0.0182948
100/137	0.00998768

TABLE 4-4

$mr_0 = 0.00001$

α	$W/2m$
65/137	0.952049
70/137	0.925341
72/137	0.897864
74/137	0.822572
75/137	0.732195
76/137	0.578074
77/137	0.383123
78/137	0.224364
79/137	0.130218
80/137	0.0790911
81/137	0.0506488
82/137	0.0340209
83/137	0.0238044
84/137	0.0172432
85/137	0.0128644

TABLE 4-5

$mr_0 = 0.000001$

α	$W/2m$
65/137	0.95181
70/137	0.920608
71/137	0.903529
72/137	0.86967
73/137	0.786053
74/137	0.573158
75/137	0.271451
76/137	0.108323
77/137	0.0480104
78/137	0.024066
79/137	0.0133224
80/137	0.00797514

TABLE 4-6

$mr_0 = 0.0000001$

α	$W/2m$
65/137	0.951695
70/137	0.915343
71/137	0.885839
72/137	0.787748
73/137	0.426903
74/137	0.10613
75/137	0.0301644
76/137	0.0110038
77/137	0.00481571
78/137	0.00240844
79/137	0.00133255
80/137	0.000797581

FIG. 4-1. Center-of-momentum energy versus field strength for a quadratic truncating potential (Crater and Van Alstine equation), keeping one term of $u_l(r)$.

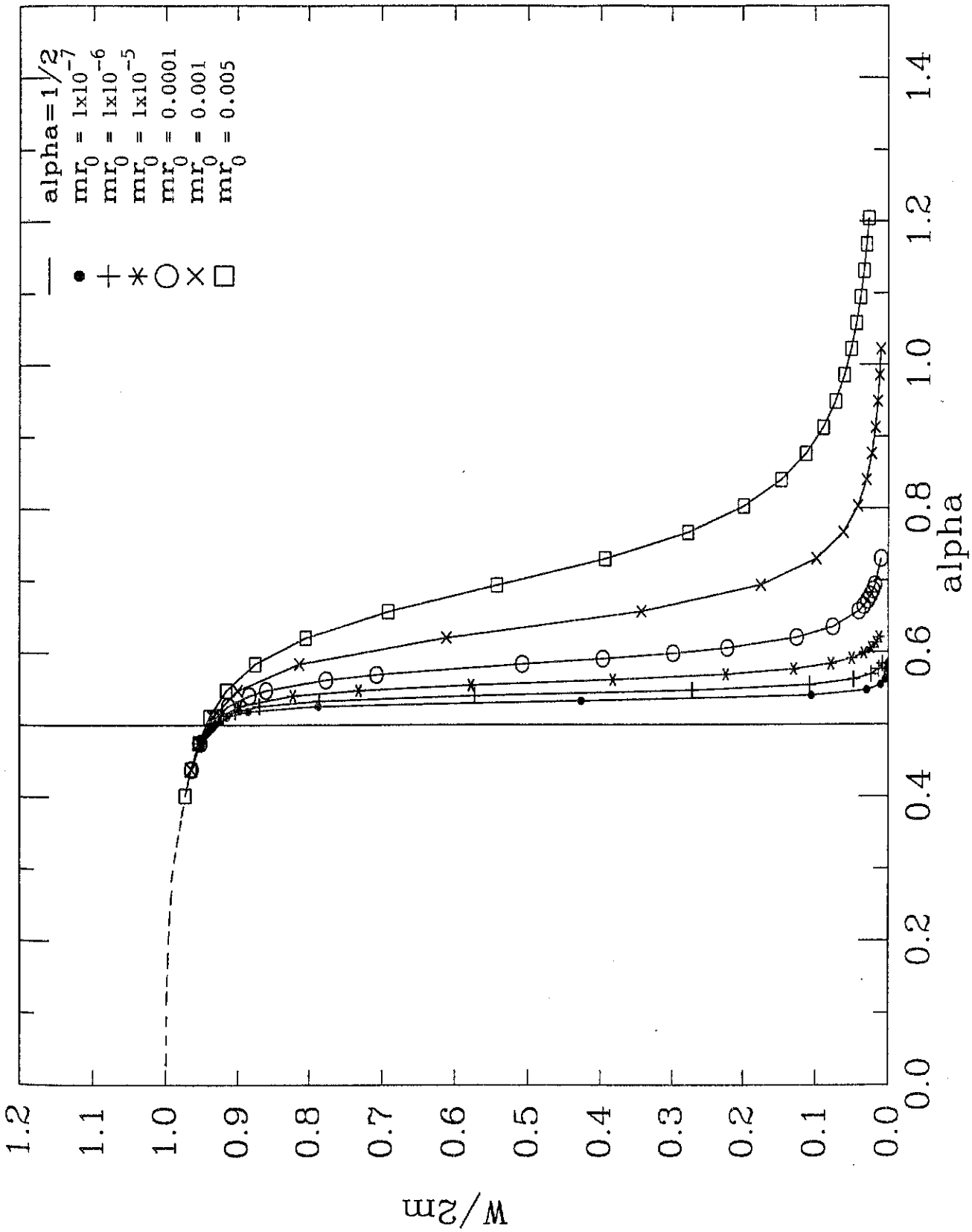


TABLE 4-7

$mr_0 = 0.005$

α	$W/2m$
55/137	0.973081
60/137	0.965036
65/137	0.953706
70/137	0.935837
75/137	0.902119
80/137	0.824251
85/137	0.646569
90/137	0.392044
95/137	0.209976
100/137	0.120174
105/137	0.0760103
110/137	0.0521879
115/137	0.038143
120/137	0.0292424
125/137	0.0232677
130/137	0.0190671
135/137	0.0160002
140/137	0.01369
145/137	0.0119036
150/137	0.0104911
155/137	0.00935269
160/137	0.00842
165/137	0.00764472

TABLE 4-8

$mr_0 = 0.001$

α	$W/2m$
60/137	0.964808
65/137	0.952858
70/137	0.932018
75/137	0.879493
80/137	0.678754
85/137	0.279088
90/137	0.0982156
95/137	0.0445379
100/137	0.02449
105/137	0.0153158
110/137	0.0104742
115/137	0.00764289
120/137	0.00585491

TABLE 4-9

$mr_0 = 0.0001$

α	$W/2m$
60/137	0.964676
65/137	0.9522
70/137	0.927145
72/137	0.904564
74/137	0.854544
75/137	0.803711
77/137	0.590685
78/137	0.432092
80/137	0.184696
81/137	0.120942
82/137	0.0819571
83/137	0.0575613
85/137	0.0311917
87/137	0.0186874
90/137	0.00994881

TABLE 4-10

$mr_0 = 0.00001$

α	$W/2m$
65/137	0.951883
70/137	0.922469
72/137	0.883289
74/137	0.715515
75/137	0.487544
76/137	0.245436
77/137	0.114925
78/137	0.0582317
79/137	0.0323122
80/137	0.0193534
81/137	0.012334
82/137	0.00826926
83/137	0.00578146
84/137	0.00418656
85/137	0.00312318

TABLE 4-11

$mr_0 = 0.000001$

α	$W/2m$
65/137	0.95173
70/137	0.917483
71/137	0.894026
72/137	0.832442
73/137	0.622604
74/137	0.241198
75/137	0.072897
76/137	0.0267204
77/137	0.0116978
78/137	0.0058494
79/137	0.00323568
80/137	0.0019363

TABLE 4-12

$mr_0 = 0.0000001$

α	$W/2m$
65/137	0.951656
70/137	0.911526
71/137	0.866057
72/137	0.629305
73/137	0.136187
74/137	0.0261812
75/137	0.00734135
76/137	0.00267456
77/137	0.00116999
78/137	0.00058497
79/137	0.000323574
80/137	0.000193631

FIG. 4-2. Center-of-momentum energy versus field strength for a quadratic truncating potential (Crater and Van Alstine equation), keeping two terms of $u_l(r)$.

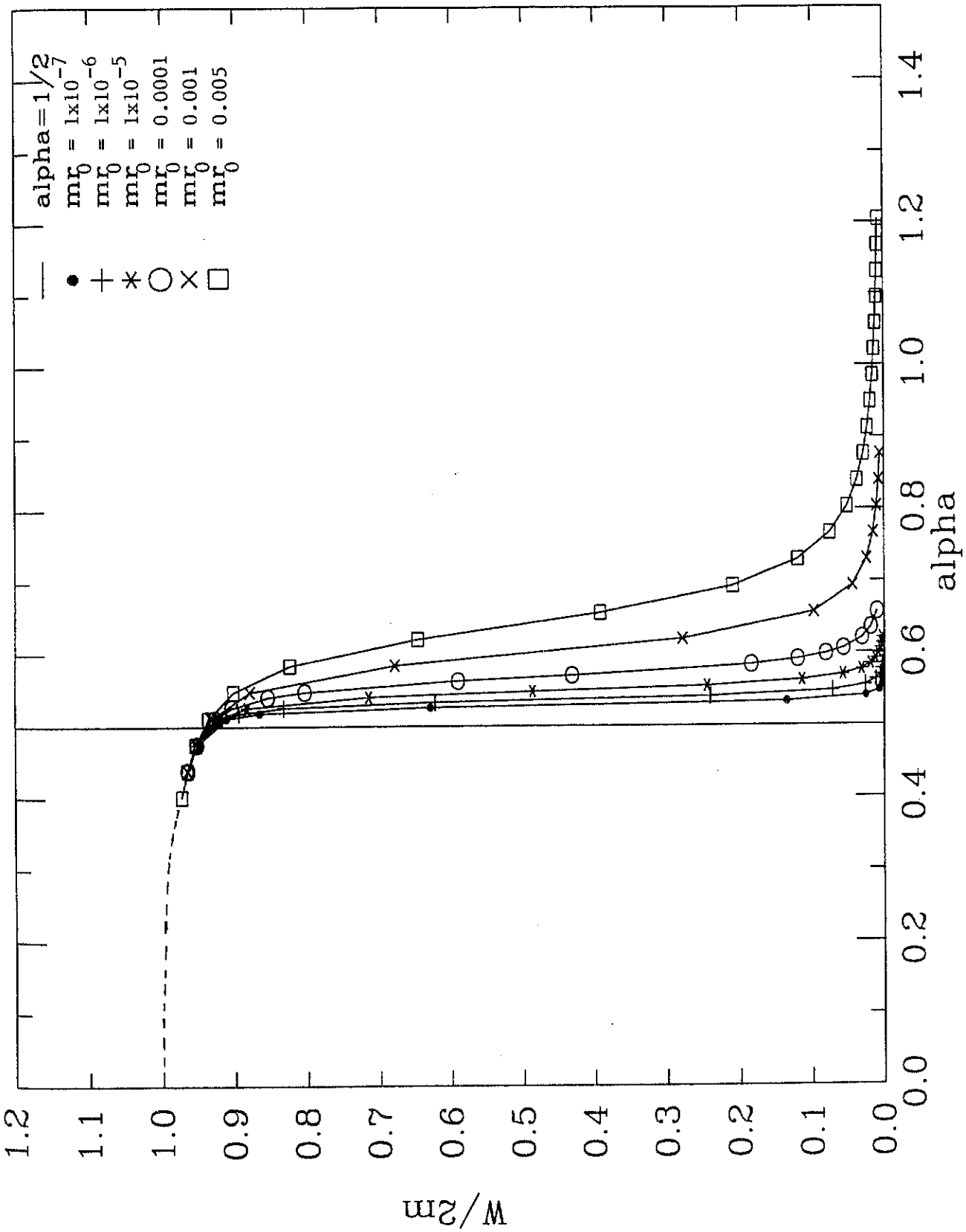


TABLE 4-13

$mr_0 = 0.005$

α	$W/2m$
55/137	0.973153
60/137	0.965245
65/137	0.954359
70/137	0.938096
75/137	0.910876
80/137	0.859659
85/137	0.760653
90/137	0.598915
95/137	0.413283
100/137	0.268586
105/137	0.178643
110/137	0.125234
115/137	0.0924373
120/137	0.0712533
125/137	0.0568965
130/137	0.0467549
135/137	0.0393369
140/137	0.0337503
145/137	0.0294383
150/137	0.0260405
155/137	0.0233155
160/137	0.0210973
165/137	0.0192687

TABLE 4-14

$mr_0 = 0.001$

α	$W/2m$
60/137	0.964905
65/137	0.953248
70/137	0.933976
75/137	0.892912
80/137	0.775596
85/137	0.493254
90/137	0.223314
95/137	0.106391
100/137	0.0592507
105/137	0.0372566
110/137	0.0255599
115/137	0.0186913
120/137	0.0143434
125/137	0.0114263
130/137	0.009377

TABLE 4-15

$mr_0 = 0.0001$

α	$W/2m$
60/137	0.964708
65/137	0.952388
70/137	0.928895
72/137	0.90995
74/137	0.874265
75/137	0.842999
77/137	0.723798
78/137	0.623075
80/137	0.371797
81/137	0.265261
82/137	0.18764
83/137	0.134576
85/137	0.0741617
87/137	0.0447185
90/137	0.0239296
91/137	0.0199834
92/137	0.0168836
93/137	0.0144151
94/137	0.0124245
95/137	0.010801
100/137	0.00595265

TABLE 4-16

$mr_0 = 0.00001$

α	$W/2m$
65/137	0.951973
70/137	0.924204
72/137	0.892819
74/137	0.791873
75/137	0.659391
76/137	0.450998
77/137	0.252578
78/137	0.135152
79/137	0.0761591
80/137	0.045869
81/137	0.0293145
82/137	0.0196918
83/137	0.0137897
84/137	0.0100003
85/137	0.00747054

TABLE 4-17

$mr_0 = 0.000001$

α	$W/2m$
65/137	0.951774
70/137	0.919396
71/137	0.900138
72/137	0.858008
73/137	0.73946
74/137	0.444954
75/137	0.166632
76/137	0.0628305
77/137	0.0276437
78/137	0.0138521
79/137	0.00767485
80/137	0.00459968

TABLE 4-18

$mr_0 = 0.0000001$

α	$W/2m$
65/137	0.951677
70/137	0.913897
71/137	0.879271
72/137	0.742554
73/137	0.290238
74/137	0.0613926
75/137	0.0173061
76/137	0.00631605
77/137	0.00276716
78/137	0.00138556
79/137	0.000767545
80/137	0.000459981

FIG. 4-3. Center-of-momentum energy versus field strength for a constant truncating potential (Crater and Van Alstine equation), keeping three terms of $u_l(r)$.

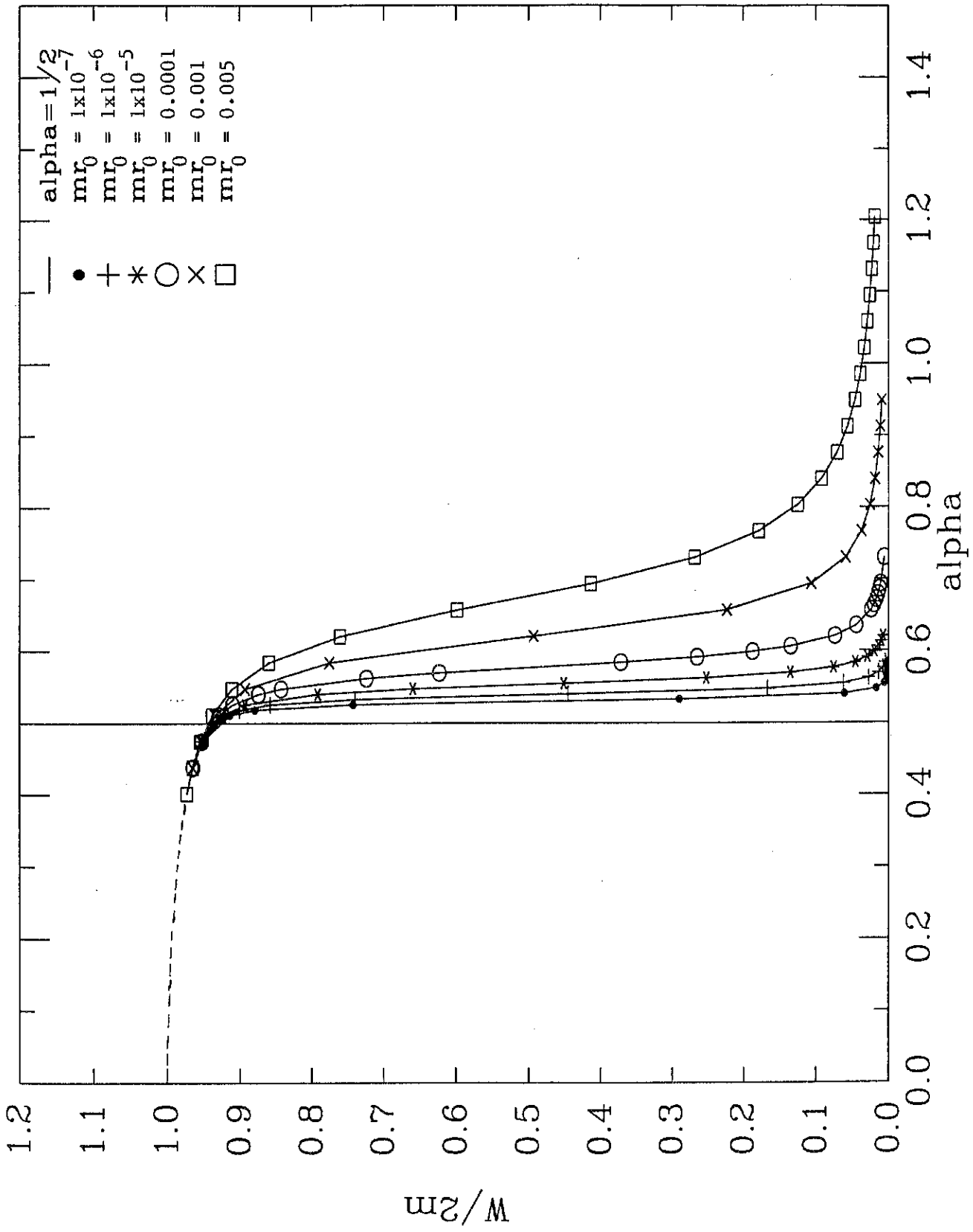
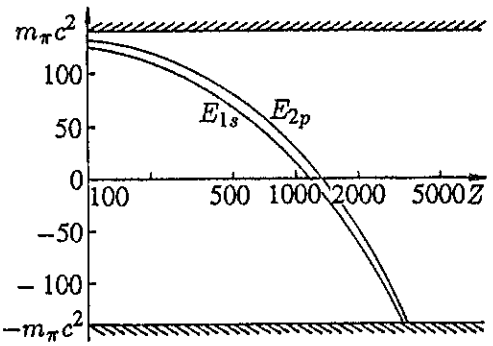


FIG. 4-4. Instability of the Klein-Gordon equation in a strong field for a quadratic truncation of the Coulomb potential (Greiner, 1990, p. 43).



Energy eigenvalues for a π^- meson in the Coulomb potential of an extended nucleus. The charge distribution of the nucleus is assumed to be a Fermi distribution [see (10)]

CHAPTER 5

MATCHING OF THE CONSTANTS

The radial Schrödinger and Klein-Gordon equations are homogeneous, second-order linear differential equations. In this chapter, a method of solving second-order linear differential equations called "matching of the constants" is introduced. The method compares a general differential equation with a known solution, to either of the radial equations. The method is of interest here because the potential of the wave equation can be left unspecified. Therefore, since the solution is assumed in advance, when a potential is found it can be deemed as an exactly solvable potential. Instead of specifying a potential and looking for a solution, the solution is specified, and the potential energy is sought.

5-1 Standard and invariant form of differential equations. A homogeneous, second-order linear differential equation in its most general form is

$$\left[F_2(x)\frac{d^2}{dx^2}+F_1(x)\frac{d}{dx}+F_0(x)\right]y(x)=0 \tag{5-1}$$

A shorter way of writing second-order differential equations will be adopted:

$$\left[F_2,F_1,F_0\right]y=0 \tag{5-2}$$

Equation (5-1) is put into standard form by dividing it through by F_2. Defining $\tilde{F}_1 \equiv F_1/F_2$ and $\tilde{F}_0 \equiv F_0/F_2$, the standard form of Eq. (5-1) in the short-hand notation is

$$\left[1,\tilde{F}_1,\tilde{F}_0\right]y=0 \tag{5-3}$$

In addition to having the function multiplying the second-order differential operator equal to one, the invariant form of a second-order differential equation also has the function multiplying the first-order differential operator equal to zero. To put Eq. (5-3) into invariant form, a substitution is made for the dependent variable y. This substitution is

$$y(x) = \exp\left[-\tfrac{1}{2}\int \tilde{F}_1\, dx\right]\psi(x) \tag{5-4}$$

The function $\tilde{F}_1$ is the first-order differential operator coefficient of Eq. (5-3). The substitution of Eq. (5-4) into Eq. (5-3), results in a new differential equation that has ψ as its dependent variable

$$[1, 0, I(x)]\,\psi = 0 \tag{5-5}$$

where

$$I(x) = \tilde{F}_0 - \left(\frac{\tilde{F}_1}{2}\right)' - \left(\frac{\tilde{F}_1}{2}\right)^2 \tag{5-6}$$

with the prime on the middle term indicating differentiation with respect to x. The function $I(x)$ is referred to as the invariant function, and Eq. (5-5) represents a differential equation in invariant form.

In future applications, a given equation in standard form will be transformed to an equation in invariant form by *computing* the invariant function with Eq. (5-6) first, and then *naming* a new dependent variable, realizing that it is related to the old dependent variable by Eq. (5-4) The usual process would be to make the appropriate variable switch first, from which the invariant form of the differential equation is derived. An example follows.

5-2 The radial Schrödinger equation in invariant form. To demonstrate Equations (5-4) and (5-6), the radial Schrödinger equation, with a central potential $V(r)$,

$$\left[\frac{-\hbar^2}{2m}\left(\frac{1}{r}\frac{d^2}{dr^2}r\right) + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r) - E\right]R(r) = 0 \tag{5-7}$$

will be written in invariant form. First, Eq. (5-7) is put into standard form:

$$\left[1, \frac{2}{r}, \frac{-\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2}V(r) + \frac{2m}{\hbar^2}E\right]R = 0 \tag{5-8}$$

To write Eq. (5-8) in invariant form, $I(r)$ is found according to Eq. (5-6), such that

$$I(r)=\frac{-\ell(\ell+1)}{r^2}-\frac{2m}{\hbar^2}V(r)+\frac{2m}{\hbar^2}E-\left(\frac{2}{2r}\right)'-\left(\frac{2}{2r}\right)^2$$

$$=\frac{-\ell(\ell+1)}{r^2}-\frac{2m}{\hbar^2}V(r)+\frac{2m}{\hbar^2}E \tag{5-9}$$

Thus, in terms of a new dependent variable, say $u(r)$, the radial Schrödinger equation in invariant form, is the familiar

$$\left[1,0,\frac{-\ell(\ell+1)}{r^2}-\frac{2m}{\hbar^2}V(r)+\frac{2m}{\hbar^2}E\right]u(r)=0 \tag{5-10}$$

where, applying Eq. (5-4), we have

$$R=\exp\left[\tfrac{-1}{2}\int\frac{2}{r}dr\right]u=\frac{1}{r}u \tag{5-11}$$

such that the relationship between the old dependent variable R, and the new variable u, is found to be $u=rR$.

With the invariant function of the radial Schrödinger equation written out explicitly in Eq. (5-9), we observe that this invariant function can be written as the sum of a function of the independent variable plus a constant. In general, if a given differential equation in the form of Eq. (5-5), has an invariant function that can be expressed as a function plus a constant, $I(x)=q(x)+\varepsilon$, and has a corresponding solution, ψ_ε, then that equation is associated with a Sturm-Liouville problem,

$$\frac{d}{dx}\left[p(x)\frac{d\psi}{dx}\right]+\left[q(x)+\lambda w(x)\right]\psi=0 \tag{5-12}$$

specifically,

$$\left[1,0,q(x)+\varepsilon\right]\psi_\varepsilon=0 \tag{5-13}$$

recognizing that $p(x)=1$, and, with $I(x)=q(x)+\varepsilon$, that the weighting function, $w(x)$, is unity. As is apparent in Eq. (5-10), the radial Schrödinger equation is also of the form of Eq. (5-13), and thus, it is recognized here as a standard example of a Sturm-Liouville problem. We will see that the method of matching of the constants involves writing other,

solved, differential equations into the form of Eq. (5-13) for the purpose of matching them with the radial Schrödinger equation.

5-3 Preliminary algebra. Before introducing the method of matching of the constants, it will be beneficial to derive a general result for later use. Assume that a solved, second-order linear differential equation, written in invariant form, is given. This given equation, with a specific invariant function and known solutions, is represented here in general terms as

$$\left[\frac{d^2}{dG^2} + I(G)\right] y(G) = 0 \tag{5-14}$$

The independent variable is G, a symbol that is used to denote that this variable is a general, initially unspecified, function of x. The requirement on the function G is that $G'(x)$ must obey the rules of weighting functions of Sturm-Liouville theory (Beker, 1990). The rule of weighting functions of Sturm-Liouville theory is that $w(x) > 0$. Weighting functions are also assumed to be real functions.

A switch in the independent variable of Eq. (5-14) is now made from G to x. The resulting differential equation will then be put into standard form and then transformed into an equation that is in invariant form. To begin this process, the chain rule of differentiation is used to find that

$$\frac{d^2}{dG^2} = \frac{1}{G'}\frac{d}{dx}\left(\frac{1}{G'}\frac{d}{dx}\right) = \frac{1}{G'^2}\frac{d^2}{dx^2} - \frac{G''}{G'^3}\frac{d}{dx} \tag{5-15}$$

The prime in Eq. (5-15) denotes differentiation with respect to x. The right-hand side of Eq. (5-15) is used to replace d^2/dG^2 in Eq. (5-14), and the subsequent differential equation, with x as its independent variable, is

$$\left[\frac{1}{G'^2}, \frac{-G''}{G'^3}, I(G)\right] y(G) = 0 \tag{5-16}$$

Before transforming Eq. (5-16) into invariant form, it is first put into standard form. Multiplying Eq. (5-16) through by G'^2, gives

$$\left[1, \frac{-G''}{G'}, G'^2 I(G)\right] y(G) = 0 \tag{5-17}$$

With Eq. (5-16) written in standard form, it is ready to be transformed to an equation that is in invariant form. Using $\tilde{F}_0 = G'^2 I(G)$ and $\tilde{F}_1 = -G''/G'$ in Eq. (5-6), the invariant function of the transformed equation, which will by denoted by $\tilde{I}(G)$, is calculated to be

$$\tilde{I}(G) = G'^2 I(G) - \left(\frac{-G''}{2G'}\right)' - \left(\frac{-G''}{2G'}\right)^2$$

$$= \frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + G'^2 I(G) \tag{5-18}$$

As an aside, Eq. (5-18) contains the Schwarzian derivative which is defined in Kulkarni (1980) as

$$\{G, x\} = \frac{G'''(x)}{G'(x)} - \frac{3}{2}\left[\frac{G''(x)}{G'(x)}\right]^2 \tag{5-19}$$

Equation (5-19) can be used to write $\tilde{I}(G)$ in a more compact form:

$$\tilde{I}(G) = \frac{1}{2}\{G, x\} + G'^2 I(G) \tag{5-20}$$

A switch is now made in the dependent variable of Eq. (5-14) from y to a new variable, ψ. Application of Eq. (5-4), using $\tilde{F}_1 = -G''/G'$, defines the relationship between the new variable ψ with the old variable y:

$$y(G) = \exp\left[\tfrac{-1}{2}\int \frac{-G''}{G'} dx\right] \psi(G) \tag{5-21}$$

Because y is assumed to be a known solution of Eq. (5-14), it is opportunistic to write ψ in terms of y. After integration and algebra in Eq. (5-21), ψ in terms of y, is found to be

$$\psi(G) = \frac{y(G)}{\sqrt{|G'|}} \tag{5-22}$$

With Equations (5-18) and (5-22) in hand, the invariant form of Eq. (5-16) can be written as

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+G'^2 I(G)\right]\frac{y(G)}{\sqrt{|G'|}}=0 \tag{5-23}$$

The prime denotes differentiation with respect to x, and G stands for $G(x)$. The beauty of Eq.(5-23) is that it is written in terms of known functions--the invariant function $I(G)$, and the solution $y(G)$ of Eq. (5-14). The function $G(x)$ is unspecified and is derived in such a way that a constant term appears in the invariant function of Eq. (5-23) for the purpose of matching this term with the constant term in the invariant function of the Schrödinger equation.

In order to use Eq. (5-23) and thus apply the method of matching of the constants, solved, second-order differential equations must be supplied. In the next section, a classification of differential equations will be discussed, leading to a handful of differential equations that will form a pool of solved equations.

5-4 Classification of differential equations. In the method of matching of the constants, a known, solved differential equation in invariant form with parameters and independent variable, $G(x)$, left unspecified, will be matched with the radial Schrödinger equation in invariant form with the energy and the potential energy left unspecified. Instead of specifying a potential and looking for a solution, the solution is specified and the potential energy is sought. The pool of solved differential equations to be matched with the Schrödinger equation and Klein-Gordon equation in the next sections, will be given.

One way to classify homogeneous, second-order linear differential equations is by the behavior of their invariant functions. Specifically, functions may be classified according to the nature (removable or essential), number and position of their singularities on the real line. The following table is a classification of differential equations based on the number and position of the singularities of the equation's invariant function (Beker, 1990). The nature of the singularities are not specified.

TABLE 5-1

#	Position	Differential Equation	Name
0	-	$[1,0,0]y=0$	—
1	0	$\left[1,\frac{A}{X},\frac{B}{X^2}\right]y=0$	Euler
2	0,1	$[x(1-x),\gamma-(1+\alpha+\beta)x,-\alpha\beta]_2F_1=0$	HGDE
2	0,"∞"	$[x,\gamma-x,-\alpha]_1F_1=0$	CHGDE

Concerning the Euler equation in Table 5-1, this equation is also called the equidimensional linear differential equation, the homogeneous linear equation, and Cauchy's equation (Hildebrand, 1976, p. 12). In addition, the abbreviations HGDE and CHGDE refer to the hypergeometric and confluent hypergeometric differential equations, respectively. CHGDE is obtained from the HGDE by a scale transformation which takes the singularity at $x=1$ to $x=\beta$ and then causes it to conflow into the singularity at $x=\infty$.

The singularities of the differential equations that are listed in the above table come from the behavior of the respective invariant functions and hence are on the finite domain. The singularity at infinity of the differential equations themselves is not part of the classification of equations in Table 5-1. This is perhaps due to the fact that the singularity at infinity is inherent in each equation.

To illustrate a singularity at infinity of a differential equation, consider the first entry in the table: $[1,0,0]y=0$. The invariant function of this equation is zero, causing the equation to be classified as having an invariant function with no singularities. However, by replacing x with $1/z$, such that

$$\frac{d^2}{dx^2}=z^4\frac{d^2}{dz^2}+2z^3\frac{d}{dz} \tag{5-26}$$

the equation $[1,0,0]y=0$ becomes

$$\frac{d^2y}{dz^2}+\frac{2}{z}\frac{dy}{dz}=0 \tag{5-27}$$

In the limit $z \to 0$, a regular singular point at $x = \infty$ becomes evident.

As a second illustration of a differential equation's singularity at infinity, consider the equation $\left[1,0,-k^2\right]y=0$. The invariant function of this equation is $-k^2$, an arbitrary constant having no singularities, thus putting the equation in the same class as $[1,0,0]y=0$ in Table 5-1. To determine the nature of the singularity of $\left[1,0,-k^2\right]y=0$ at infinity, the dependent variable is switched from x to $1/z$, leading to

$$\left[\frac{d^2}{dz^2}+\frac{2}{z}\frac{d}{dz}-\frac{k^2}{z^4}\right]y=0 \tag{5-28}$$

In the limit $z \to 0$, an *irregular* singular point at $x = \infty$ becomes evident, and distinguishes $\left[1,0,-k^2\right]y=0$ from $[1,0,0]y=0$.

Table 5-2 is constructed from a summary of solved second-order differential equations that are classified according to their singularities (Morse, 1953, pp. 667-74). Unlike Table 5-1, Table 5-2, which is found at the end of this section, takes into account all of an equation's singularities, not just those of its invariant function, and states whether a singularity is regular or irregular. Thus, the equation $\left[1,0,-k^2\right]y=0$, noticeably missing in Table 5-1, is now distinguished from $[1,0,0]y=0$, and appears in Table 5-2.

The purpose of Table 5-2 is to assemble solved second-order differential equations that can be used in conjunction with the radial Schrödinger and Klein-Gordon equations in the method of matching of the constants. It is not the intention in constructing Table 5-2 to limit future study to only these six equations.

The first three equations, transformed to an equation in the form of Eq. (5-23), have all led to deriving a constant potential when matched with the Schrödinger equation. The Mathieu equation will be used to conclude this chapter as a means of demonstrating Eq. (5-23), and the method of matching of the constants. The confluent hypergeometric and hypergeometric differential equations are the focus of later chapters.

TABLE 5-2

Regular Singular Points	Irregular Singular Points	Differential Equation	Name
One: ∞	None	$[1,0,0]y=0$	—
None	One: ∞	$\left[1,0,-k^2\right]y=0$	Linear Oscillator if k is imaginary
Two: $0,\infty$	None	$\left[1,\frac{A}{X},\frac{B}{X^2}\right]y=0$	Euler
None	Two: $0,\infty$	$[1,0,a-2q\cos 2x]y(x)=0$	Mathieu
Three: $0,1,\infty$	None	$\left[x(1-x),\gamma-(1+\alpha+\beta)x,-\alpha\beta\right]_2F_1=0$	HGDE
One: 0	One: ∞	$\left[x,\gamma-x,-\alpha\right]_1F_1=0$	CHGDE

5-5 Mathieu equation. To demonstrate the method of matching of the constants, a generalized Mathieu differential equation will be derived and matched with the radial Schrödinger equation.

The Mathieu differential equation is

$$[1,0,a-2q\cos 2x]y(x)=0 \tag{5-29}$$

The solution to Eq. (5-29) is the Mathieu function, denoted here by $y(x)$. Properties of Mathieu functions can be found in Abramowitz (1972).

The independent variable x in Eq. (5-29) is now taken to be a function, say $x=G(r)$, and a switch in independent variables from G to r is promptly made. Since Eq. (5-29) is already in invariant form, the resulting equation from our switch is derived by substituting the invariant function and solution of Eq. (5-29) into Eq. (5-23),

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+G'^2I(G)\right]\frac{y(G)}{\sqrt{|G'|}}=0 \tag{5-23}$$

as follows,

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+G'^2a-G'^2 2q\cos 2G\right]\frac{y(G)}{\sqrt{|G'|}}=0 \tag{5-30}$$

Equation (5-30) is the generalized Mathieu equation which we now match with the radial Schrödinger equation, Eq. (5-10):

$$\left[1,0,\frac{-\ell(\ell+1)}{r^2}-\frac{2m}{\hbar^2}V(r)+\frac{2m}{\hbar^2}E\right]u(r)=0 \tag{5-10}$$

In anticipation of matching of the constants, the presence of the energy term in Eq. (5-10) requires $G(r)$ to be chosen such that a constant term also appears in the invariant function of Eq. (5-30). One simple condition on $G(r)$ in which a constant term is obtained is to demand that G'^2 = a constant. According to this condition, we choose $G=c_1r+c_2$, where c_1 and c_2 are arbitrary constants. Furthermore, we set $c_2=0$, and with $G=c_1r$, the invariant function of Eq. (5-30) becomes

$$I(r)=c_1^{\,2}a-c_1^{\,2}2q\cos 2c_1r \tag{5-31}$$

The terms of Eq. (5-31) can be matched with the terms of Eq. (5-10) as follows:

$$\frac{-\ell(\ell+1)}{r^2}=0 \tag{5-32a}$$

$$-\frac{2mV(r)}{\hbar^2}=-c_1^{\,2}2q\cos 2c_1r \tag{5-32b}$$

$$\frac{2mE}{\hbar^2}=c_1^{\,2}a \tag{5-32c}$$

The first of these equations, Eq. (5-32a), suggests that we set $\ell=0$. Upon taking $\ell=0$ in this and other such problems, the Morse potential for example, Eq. (5-10) may from that time forward be considered as the one-dimensional Schrödinger equation. In such cases, it becomes appropriate to replace r with x as the symbol for the independent variable, and to denote the eigenfunction as $\varphi(x)$ instead of $u(r)$. With this in mind, Eq. (5-32b) can be rearranged such that

$$\frac{V(x)}{2\cos 2c_1 x} = \frac{c_1^2 q\hbar^2}{2m} \tag{5-33}$$

With the left-hand side of Eq. (5-33) equated to a separation constant, defined as V_0, the potential energy is derived:

$$V(x) = 2V_0 \cos 2c_1 x \tag{5-34}$$

Finally, an expression for energy is obtained from Eq. (5-32c). We find that

$$E = \frac{\hbar^2}{2m} c_1^2 a \tag{5-35}$$

By equating the right-hand side of Eq. (5-33) to V_0 and solving for c_1^2, the energy in terms of V_0 is

$$E = V_0 \frac{a}{q} \tag{5-36}$$

Quantization of energy is found by selecting parameters that lead to square integrable eigenfunctions. The unnormalized eigenfunction is obtained merely by reading it off from Eq. (5-30). Thus, with $G = c_1 x$, we find that

$$\varphi(x) = \frac{y(c_1 x)}{\sqrt{|c_1|}} \tag{5-37}$$

Equation (5-37) is unnormalized and $y(c_1 x)$ is a Mathieu function.

We do not pursue this problem any further (Liboff, 1980, p. 576) since our goal here was to demonstrate the method of matching of the constants by deriving an exactly solvable potential, Eq. (5-34). The derivation of Eq. (5-34) is in itself significant because it was derived without any prior knowledge of its existence on our part which suggests that the method of matching of the constants can uncover unexpected exactly solvable potentials. On the other hand, attention is now turned to deriving potentials that are expected from the outset. This will allow us to gain experience with the method of matching of the constants, quantization of energy will be demonstrated in most of the cases, for the ultimate purpose

of using this experience to derive an exactly solvable potential that may be used as a truncating potential in the study of strongly coupled positronium.

CHAPTER 6

CONFLUENT HYPERGEOMETRIC EQUATION

The method of matching the constants is used to match the radial Schrödinger equation with an equation that starts out as the confluent hypergeometric differential equation (CHGDE). Three potentials will be derived--the Coulomb potential, the harmonic oscillator potential, and the Morse potential for $\ell = 0$.

6-1 Confluent hypergeometric equation. To further demonstrate the method of matching of the constants, the invariant function of a generalized confluent hypergeometric differential equation will be matched with the invariant function of the radial Schrödinger equation.

The confluent hypergeometric equation, CHGDE, is

$$\left[x, \gamma - x, -\alpha\right]_1 F_1(\alpha, \gamma; x) = 0 \tag{6-1}$$

The solution of Eq. (6-1), denoted by ${}_1F_1(\alpha, \gamma; x)$, is the confluent hypergeometric function, or Kummer's function (Abramowitz, 1972, p. 504), a series of the form

$${}_1F_1(\alpha, \gamma; x) = 1 + \frac{\alpha}{\gamma}\frac{x}{1!} + \frac{\alpha(\alpha+1)}{\gamma(\gamma+1)}\frac{x^2}{2!} + \ldots \tag{6-2}$$

In Eq. (6-2), $\gamma = 0, -1, -2, \ldots$ will not be allowed. Furthermore, if $\alpha = 0, -1, -2, \ldots$, then, the otherwise infinite series of Eq. (6-2), truncates into a polynomial. A definition is made for convenience, $\nu \equiv -\alpha$, and for future reference, Eq. (6-1) has square integrable solutions for $\nu = 0, 1, 2, \ldots$ (Beker, 1990).

The standard form of Eq. (6-1) is

$$\left[1, \frac{\gamma - x}{x}, \frac{\nu}{x}\right]_1 F_1(-\nu, \gamma; x) = 0 \tag{6-3}$$

Using Eq. (6-3) as a starting point, an equation that is in invariant form will now be derived. The invariant function of this equation is calculated by applying Eq. (5-6), leading to

$$I(x)=\frac{\nu}{x}-\left(\frac{\gamma-x}{2x}\right)'-\left(\frac{\gamma-x}{2x}\right)^2$$

$$=\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{1}{x^2}+\left(\frac{\gamma}{2}+\nu\right)\frac{1}{x}-\frac{1}{4} \tag{6-4}$$

Deriving Eq. (6-4) presupposes that a switch has been made, in accordance with Eq. (5-4), in the dependent variable of Eq. (6-3). Defining the new dependent variable as $\psi(x)$, we now make the switch, such that

$${}_1F_1(-\nu,\gamma;x)=\exp\left[-\tfrac{1}{2}\int\frac{\gamma-x}{x}dx\right]\psi(x) \tag{6-5}$$

Integrating, and finding $\psi(x)$ in terms of ${}_1F_1(-\nu,\gamma;x)$, leads to

$$\psi(x)=e^{-x/2}x^{\gamma/2}\,{}_1F_1(-\nu,\gamma;x) \tag{6-6}$$

Substituting Eqs. (6-4) and (6-6) into Eq. (5-5) gives the CHGDE written in invariant form as

$$\left[1,0,\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{1}{x^2}+\left(\frac{\gamma}{2}+\nu\right)\frac{1}{x}-\frac{1}{4}\right]e^{x/2}x^{\gamma/2}\,{}_1F_1(-\nu,\gamma;x)=0 \tag{6-7}$$

At this point, it is desired that the independent variable, x, is taken to be a function, $G(r)$. The algebra required to change independent variables from G to r in a second-order differential equation was the subject of Sec. 5-3 in the previous chapter, and produced Eq. (5-23) as a general equation for making this switch. Applying Eq. (5-23) by substituting Eqs. (6-4) and (6-6), as the invariant function and the solution, respectively, results in the following equation, referred to as Eq. (6-8):

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{G'^2}{G^2}+\left(\frac{\gamma}{2}+\nu\right)\frac{G'^2}{G}-\frac{1}{4}G'^2\right]\frac{e^{-G/2}G^{\gamma/2}}{\sqrt{|G'|}}\,{}_1F_1(-\nu,\gamma;G)=0 \tag{6-8}$$

The prime in this equation indicates differentiation with respect to r.

Equation (6-8) is matched with the radial Schrödinger equation, and later, with the radial Klein-Gordon equation, in deriving exactly solvable potentials whose eigenfunctions involve the confluent hypergeometric function. Its importance cannot be emphasized enough, as it is the starting point for research beyond what is given in this work.

Matching terms of the invariant function of Eq. (6-8) with terms of the invariant function of the radial Schrödinger equation, requires the presence of a constant term in the invariant function of Eq. (6-8). Obtaining a constant term is accomplished in the judicious selection of the unknown function $G(r)$. The selection of $G(r)$ that leads to the derivation of the Coulomb potential, the subject of the next section, is made by solving the differential equation G'^2 = constant. Two other conditions on $G(r)$, also in the form of differential equations, are the subjects of the following sections.

6-2 Coulomb potential. Equation (6-8),

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{G'^2}{G^2}+\left(\frac{\gamma}{2}+\nu\right)\frac{G'^2}{G}-\frac{1}{4}G'^2\right]\frac{e^{-G/2}G^{\gamma/2}}{\sqrt{|G'|}}\,{}_1F_1(-\nu,\gamma;G)=0 \tag{6-8}$$

is to be matched with the radial Schrödinger equation,

$$\left[1,0,\frac{-\ell(\ell+1)}{r^2}-\frac{2m}{\hbar^2}V(r)+\frac{2m}{\hbar^2}E\right]u=0 \tag{5-10}$$

by requiring that $G(r)$ satisfy the condition G'^2 = constant. The general solution to such an equation is $G=\pm c_1 r+c_2$, where c_1 and c_2 are constants. The constant c_2 is set equal to zero and a choice is made to keep the positive sign in front of c_1, which leads to a $G=c_1 r$.

With $G=c_1 r$, the invariant function of Eq. (6-8) is calculated as

$$I(r)=\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{1}{r^2}+\left(\frac{\gamma}{2}+\nu\right)\frac{c_1}{r}-\frac{c_1^2}{4} \tag{6-9}$$

Equation (6-9) is now matched with the invariant function of the radial Schrödinger equation. The constant terms, and the $1/r^2$ terms, match, respectively, as follows:

$$\frac{2mE}{\hbar^2} = \frac{-c_1^2}{4} \tag{6-10}$$

$$\frac{-\ell(\ell+1)}{r^2} = \left(\frac{\gamma}{2} - \frac{\gamma^2}{4}\right)\frac{1}{r^2} \tag{6-11}$$

The $1/r$ term of Eq. (6-9), matched with the $V(r)$ term of the Schrödinger equation, gives

$$\frac{-2mV(r)}{\hbar^2} = \left(\frac{\gamma}{2} + \nu\right)\frac{c_1}{r} \tag{6-12}$$

As we begin to analyze Eqs. (6-10) through (6-12), the following quadratic equation in γ is obtained from Eq. (6-11):

$$\gamma^2 - 2\gamma - 4\ell(\ell+1) = 0 \tag{6-13}$$

The roots of this quadratic equation are $\gamma = 2(\ell+1)$ and -2ℓ. The positive root is chosen over the negative root. This choice is made because the factor of $G^{\gamma/2}$ in the solution of Eq. (6-8), where $G = c_1 r$, would blow up at $r = 0$ for $\gamma = -2\ell$.

Substitution of $\gamma = 2(\ell+1)$ is now made into Eq. (6-12). After the constant factors are separated from the two factors that have r dependence, the following equality is derived:

$$-rV(r) = \frac{\hbar^2}{2m}(\ell+1+\nu)c_1 \tag{6-14}$$

The right-hand side of Eq. (6-14) is constant; therefore, the left-hand side of the equation is also equal to a constant. In anticipation of solving for the Coulomb potential, the separation constant is called e^2. Setting $-rV(r) = e^2$, the potential energy is derived:

$$V(r) = \frac{-e^2}{r} \tag{6-15}$$

The energy is found, simply enough, from Eq. (6-10):

$$E = \frac{-\hbar^2}{2m}\frac{c_1^2}{4} \tag{6-16}$$

The constant c_1 is determined by setting the right-hand side of Eq. (6-14) equal to e^2. After algebra, we have

$$c_1 = \frac{2me^2}{\hbar^2(\ell+1+\nu)} \tag{6-17}$$

Substituting Eq. (6-17) into Eq. (6-16), gives the energy as

$$E = \frac{-me^4}{2\hbar^2(\ell+1+\nu)^2} \tag{6-18}$$

To determine quantization of energy, the eigenfunction is now considered. The unnormalized eigenfunction, from Eq. (6-8), is

$$u(r) = \frac{e^{-G/2}G^{\gamma/2}}{\sqrt{|G'|}}\,{}_1F_1(-\nu,\gamma;G) \tag{6-19}$$

Recall that for $\nu = 0,1,2,\ldots$, that the CHGDE had square integrable solutions and therefore, ν is now defined here as such. Furthermore, if we define $n = (\ell+1+\nu)$, leading to $\nu = n-(\ell+1)$, then we demand that $n \geq (\ell+1)$. In addition, since the smallest value of ℓ is zero, we note that $n = 1,2,3,\ldots$ is required.

With the definition that $n = (\ell+1+\nu)$, the energy is rewritten as

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \tag{6-20}$$

and Eq. (6-19), the unnormalized radial eigenfunction (recalling too that $G = c_1 r$) is rewritten as

$$u(r) = \frac{e^{\frac{-c_1 r}{2}}(c_1 r)^{\ell+1}}{\sqrt{c_1}}\,{}_1F_1\left(-\{n-(\ell+1)\},2\ell+2;c_1 r\right) \tag{6-21}$$

with $c_1 = 2me^2/n\hbar^2$.

Finally, to finish this section, the confluent hypergeometric function can be found in terms of the associated Laguerre function from the following relationship:

$$L_n^m(x) = \frac{(n+m)!}{n!m!}\,{}_1F_1(-n, m+1; x) \tag{6-22}$$

(Arfken, 1985, p. 755). Therefore, putting Eq. (6-19) in terms of the associated Laguerre function, the final form of our eigenfunction is

$$u_{nl}(r) = A_{nl}\, e^{\frac{-c_1 r}{2}} (c_1 r)^{l+1} L_{n-l-1}^{2l+1}(c_1 r) \tag{6-23}$$

The constant c_1 is given in Eq. (6-17), and A_{nl} is a normalization factor (Liboff, 1980, p. 397). We recognize, thus, the energy, Eq. (6-20), and the wave function, Eq. (6-23), of the Schrödinger hydrogen atom, as we now turn our attention to the harmonic oscillator potential.

6-3 Harmonic oscillator potential. Equation (6-8),

$$\left[1, 0, \frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + \left(\frac{\gamma}{2} - \frac{\gamma^2}{4}\right)\frac{G'^2}{G^2} + \left(\frac{\gamma}{2} + \nu\right)\frac{G'^2}{G} - \frac{1}{4}G'^2\right] \frac{e^{-G/2} G^{\gamma/2}}{\sqrt{|G'|}}\, {}_1F_1(-\nu, \gamma; G) = 0 \tag{6-8}$$

is again to be matched with the radial Schrödinger equation,

$$\left[1, 0, \frac{-\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2}V(r) + \frac{2m}{\hbar^2}E\right]u = 0 \tag{5-10}$$

In this section, however, the condition on G that will provide a constant term in the invariant function of Eq. (6-8), is G'^2/G= constant. The equation

$$\frac{G'^2}{G} = c_1^2 \tag{6-24}$$

where c_1 is an arbitrary real constant, can be written as

$$\int \frac{dG}{\sqrt{G}} = \int \pm c_1 \, dr \tag{6-25}$$

which leads to

$$G = \frac{\left(\pm c_1 r + c_2\right)^2}{4} \tag{6-26}$$

The integration constant c_2 is chosen to be zero, and for convenience, we define $A \equiv c_1^2/4$, and thus we have

$$G(r) = Ar^2 \tag{6-27}$$

Equation (6-27) is used to calculate the invariant function of Eq. (6-8) in terms of r. The result of the calculation is

$$I(r) = \left(\frac{-3}{4} + 2\gamma - \gamma^2\right)\frac{1}{r^2} + \left(\frac{\gamma}{2} + \nu\right)4A - A^2 r^2 \tag{6-28}$$

The terms of Eq. (6-28) are promptly matched with the terms of Eq. (5-10). We find that

$$\frac{-3}{4} + 2\gamma - \gamma^2 = -\ell(\ell+1) \tag{6-29}$$

$$-A^2 r^2 = \frac{-2mV(r)}{\hbar^2} \tag{6-30}$$

$$\left(\frac{\gamma}{2} + \nu\right)4A = \frac{2mE}{\hbar^2} \tag{6-31}$$

Equation (6-29) is a quadratic equation in γ whose roots are

$$\gamma = \ell + \frac{3}{2} \text{ and } \gamma = -\ell + \frac{1}{2} \tag{6-32}$$

The second value for γ, $-\ell + \frac{1}{2}$, causes the solution of Eq. (6-8) to blow up at $r = 0$ for all values of ℓ with the exception of $\ell = 0$. Both roots, with $\ell = 0$, are valid and lead to odd and even Hermite polynomials, respectively, as solutions to Eq. (6-8) for this choice of G.

Equation (6-30) is rearranged as

$$\frac{2V(r)}{r^2} = \frac{A^2\hbar^2}{m} \tag{6-33}$$

A separation constant, which anticipates deriving the harmonic oscillator potential, is defined as $\omega^2 m$. The right-hand side of Eq.(6-33), when equated with the separation constant, gives the potential energy as

$$V(r) = \frac{1}{2}\omega^2 m r^2 \tag{6-34}$$

The left-hand side of Eq. (6-33), when equated to the separation constant, gives the constant A as

$$A = \frac{m\omega}{\hbar} \tag{6-35}$$

To derive the energy, Eq. (6-35) is substituted into Eq. (6-31), and solving for E leads to

$$E = \hbar\omega(2\nu + \gamma) \tag{6-36a}$$

$$E = \hbar\omega\left(2\nu + \ell + \tfrac{3}{2}\right) \text{ with } \gamma = \ell + \frac{3}{2} \tag{6-36b}$$

$$E = \hbar\omega\left(2\nu + \tfrac{1}{2}\right) \text{ with } \gamma = \frac{1}{2} \tag{6-36c}$$

Having derived the potential and the energy, the eigenfunction will now be considered to determine quantization of energy. The general form of the eigenfunction of Eq. (6-8) is

$$u(r) = \frac{e^{-G/2} G^{\gamma/2}}{\sqrt{|G'|}} {}_1F_1(-\nu, \gamma; G) \tag{6-37}$$

Substituting $G = Ar^2$ along with $\gamma = \ell + 3/2$ into Eq. (6-37), and after some algebra, we find that the radial eigenfunction can be rewritten as

$$u(r) = N e^{\frac{-Ar^2}{2}} \left(Ar^2\right)^{\frac{\ell+1}{2}} {}_1F_1\left(-\nu, \ell+\tfrac{3}{2}; Ar^2\right) \tag{6-38}$$

N is a normalizing constant into which most of the previous constant factors have been absorbed. In order have Eq. (6-38) square integrable, we demand that $\nu = 0,1,2,\ldots$, a requirement that also means the energy, Eq. (6-36b), is quantized. However, we choose to write the energy and radial eigenfunction in terms of n, such that $n = 2\nu + \ell$. Under the restriction on ν, $\nu = 0,1,2,\ldots$, we see that $n \geq \ell$. Finally, the energy and the radial eigenfunction in terms of n are

$$E = \hbar\omega\left(n + \tfrac{3}{2}\right) \tag{6-39}$$

and

$$u(r) = N e^{\frac{-Ar^2}{2}} \left(Ar^2\right)^{\frac{\ell+1}{2}} {}_1F_1\left(-\tfrac{1}{2}(n-\ell), \ell+\tfrac{3}{2}; Ar^2\right) \tag{6-40}$$

keeping in mind that $A = m\omega/\hbar$ and N is a normalization constant in Eq. (6-40).

If we return to Eq. (6-32) and set $\ell = 0$, then the values of γ are $\frac{3}{2}$ or $\frac{1}{2}$. These roots lead to odd and even Hermite polynomials, and this derivation is included here to end this section.

With $\ell = 0$, it is preferable in this problem to think of Eq. (5-10) as the one dimensional Schrödinger equation and replace r with x in Eqs. (6-8) and (5-10), and $u(r)$ with $\varphi(x)$ in Eq. (5-10). With these replacements in mind, Eq. (6-38) would be derived as

$$\varphi(x) = N e^{\frac{-Ax^2}{2}} \sqrt{A}x \, {}_1F_1\left(-\nu, \tfrac{3}{2}; Ax^2\right) \tag{6-41}$$

Again, in order to have a square integrable eigenfunction, we demand that $\nu = 0,1,2,\ldots$. Furthermore, Eq. (6-41) compares favorably with the following relationship between odd Hermite polynomials and the confluent hypergeometric function (Arfken, 1985, p. 755):

$$H_{2n+1}(x) = (-1)^n \frac{2(2n+1)!}{(n)!} x \, {}_1F_1\left(-n, \tfrac{3}{2}; x^2\right) \tag{6-42}$$

Therefore, Eq. (6-41), again keeping in mind that $A = m\omega/\hbar$ and N is a normalization constant, can be rewritten as

$$\varphi(x) = Ne^{\frac{-Ax^2}{2}} H_{2v+1}\left(\sqrt{A}x\right) \tag{6-43}$$

and the energy, Eq. (6-36b), can be recast as

$$E = \hbar\omega\left((2v+1)+1/2\right) \tag{6-44}$$

To recover the even Hermite polynomials, $\gamma = \frac{1}{2}$ is substituted in Eq. (6-37), with $G = Ax^2$, leading to

$$\varphi(x) = N\, e^{\frac{-Ax^2}{2}}\, {}_1F_1\left(-v, \tfrac{1}{2}; Ax^2\right) \tag{6-45}$$

Once again, to have a square integrable eigenfunction, we require that $v = 0,1,2,\ldots$. The relationship between even Hermite polynomials and the confluent hypergeometric equation is

$$H_{2n}(x) = (-1)^n \frac{(2n)!}{n!}\, {}_1F_1\left(-n, \tfrac{1}{2}; x^2\right) \tag{6-46}$$

(Arfken, 1985, p. 755). Therefore, Eq. (6-45) can be written as

$$\varphi(x) = N\, e^{\frac{-Ax^2}{2}}\, H_{2v}\left(\sqrt{A}x\right) \tag{6-47}$$

with $A = m\omega/\hbar$ and N, a normalization constant. The energy remains unchanged from Eq. (6-36c), $E = \left(2v+1/2\right)$.

To end this section, and for comparison's sake with Liboff (1980, p. 189), the energy of the one-dimensional harmonic oscillator is

$$E_n = \left(n+1/2\right) \text{ for } n = 0,1,2,\ldots \tag{6-48}$$

the eigenfunction is

$$\psi_n(x) = A_n\, e^{\frac{-m\omega}{2\hbar}x^2}\, H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \tag{6-49}$$

and the normalizing factor is given as

$$A_n = \left(\frac{1}{2^n n!} \sqrt{\frac{m\omega}{\hbar\pi}} \right)^{1/2} \tag{6-50}$$

6-4 Morse potential. In this section, the Morse potential will be derived using the method of matching of the constants. For reference, Eq. (6-8) and the radial Schrödinger equation are restated here:

$$\left[1, 0, \frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + \left(\frac{\gamma}{2} - \frac{\gamma^2}{4}\right)\frac{G'^2}{G^2} + \left(\frac{\gamma}{2} + \nu\right)\frac{G'^2}{G} - \frac{1}{4}G'^2 \right] \frac{e^{-G/2} G^{\gamma/2}}{\sqrt{|G'|}} \, {}_1F_1(-\nu, \gamma; G) = 0$$

$$\left[1, 0, \frac{-\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2}V(r) + \frac{2m}{\hbar^2}E \right] u = 0 \tag{5-10}$$

The Morse potential will be derived under this condition on $G(r)$:

$$\frac{G'^2}{G^2} = c_1^2 \tag{6-51}$$

where c_1 is a real, positive constant. Equation (6-51) is equivalent to

$$\int \frac{dG}{G} = \int \pm c_1 \, dr \tag{6-52}$$

an equation from which G is found. Integrating Eq. (6-52) gives

$$\ln|G| = \pm c_1 r + c_2 \tag{6-53}$$

leading to one choice of G, namely

$$G = e^{c_2} e^{\pm c_1 r} = A e^{-ar} \tag{6-54}$$

where these definitions are used: $A = e^{c_2}$ and $a = c_1$. We are keeping the negative sign instead of the positive sign as the factor originally found multiplying c_1, knowing that this choice leads to deriving the Morse potential.

The higher derivatives of G are now calculated and substituted into Eq. (6-8). The invariant equation of Eq. (6-8) becomes

$$I(r)=\left(\frac{-1}{4}+\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)a^2+\left(\frac{\gamma}{2}+\nu\right)a^2Ae^{-ar}-\frac{a^2A^2e^{-2ar}}{4} \tag{6-55}$$

Furthermore, adding and subtracting a constant term to Eq. (6-55) is an option that is exercised in this problem in order to derive a Morse potential that is in keeping with Johnson (1986, p. 319). Since we have not exercised this option in previous examples, this section now illustrates a new flexibility that one should keep in mind when using the method of matching of the constants.

The constant term is defined has $Ca^2/4$, and Eq. (6-55) becomes

$$I(r)=\left(\frac{-1}{4}+\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)a^2+\left(\frac{\gamma}{2}+\nu\right)a^2Ae^{-ar}-\frac{a^2A^2e^{-2ar}}{4}+\frac{Ca^2}{4}-\frac{Ca^2}{4} \tag{6-56}$$

In matching Eq. (6-56) with the invariant function of Eq. (5-10), we first set $\ell=0$ in Eq. (5-10). In so doing, we treat this as a one-dimensional problem with $-\infty<r<\infty$. The next step, then, is to match the constant terms of the two invariant functions:

$$\frac{2mE}{\hbar^2}=\left(\frac{-1}{4}+\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)a^2+\frac{Ca^2}{4} \tag{6-57}$$

The potential energy term of Eq. (5-10) is matched below with all of the remaining terms of Eq. (6-56):

$$\frac{-2mV(r)}{\hbar^2}=\left(\frac{\gamma}{2}+\nu\right)a^2Ae^{-ar}-\frac{a^2A^2e^{-2ar}}{4}-\frac{Ca^2}{4} \tag{6-58}$$

Equation (6-58) is solved for the potential, leading to

$$V(r)=\frac{\hbar^2a^2}{8m}\left\{A^2e^{-2ar}-2(\gamma+2\nu)Ae^{-ar}+C\right\} \tag{6-59}$$

At this point we could claim success in deriving the Morse potential. However, Eq. (6-59) will now be put into a form that compares more closely with Johnson (1986).

In order to specify the constant A, the particular value of r, which shall be called r_e, that corresponds to the minimum value of the potential, is found. We take the derivative of Eq. (6-59), set it equal to zero, and then solve for r_e. In mathematical terms, from the equation

$$\left.\frac{dV}{dr}\right|_{r=r_e} = \frac{\hbar^2 a^2}{8m}\left\{-2aA^2e^{-2ar} + 2a(\gamma+2\nu)Ae^{-ar}\right\}\Big|_{r=r_e} = 0 \tag{6-60}$$

it is derived that

$$r_e = \frac{1}{a}\ln\left|\frac{A}{\gamma+2\nu}\right| \tag{6-61}$$

Solving Eq. (6-61) for A leads to $A = (\gamma+2\nu)e^{ar_e}$, an expression which is promptly substituted into Eq. (6-59), resulting in the following equation:

$$V(r) = \frac{\hbar^2 a^2}{8m}\left\{(\gamma+2\nu)^2 e^{-2a(r-r_e)} - 2(\gamma+2\nu)^2 e^{-a(r-r_e)} + C\right\} \tag{6-62}$$

If constant C is chosen such that $C = (\gamma+2\nu)^2$, then Eq. (6-62) becomes

$$V(r) = D\left\{e^{-a(r-r_e)} - 1\right\}^2 \tag{6-63}$$

where D is a positive, real constant defined as

$$D = \frac{\hbar^2 a^2}{8m}(\gamma+2\nu)^2 \tag{6-64}$$

Equation (6-63) is the Morse potential in the form matching Johnson (1986, p. 319).

Next, the energy derived from Eq. (6-57) is

$$E = \frac{\hbar^2 a^2}{8m}\left(-1+2\gamma-\gamma^2+C\right) \tag{6-65}$$

After some algebra and using $C = (\gamma+2\nu)^2$, Eq. (6-65) can be written as

$$E = \frac{\hbar^2 a^2}{2m}(v+1/2)(\gamma + v - 1/2) \tag{6-66}$$

From Eq. (6-64), the parameter γ can be expressed in terms v and the constant D. Therefore, for a given D, Eq. (6-66) depends only on v, and if the requirement $v = 0,1,2,\ldots$ is to be imposed as a consequence of requiring the eigenfunction to be square integrable, as it has been in the first two examples of this chapter, then the energy, Eq. (6-66), will be quantized. The eigenfunction is now considered.

The general form of the eigenfunction is read off from Eq. (6-8) and in this case with

$$G(r) = Ae^{-ar} = (\gamma + 2v)e^{-a(r-r_e)} \tag{6-67}$$

the eigenfunction, with N introduced as the normalization factor, becomes

$$u(r) = N\exp\left[\frac{-(\gamma+2v)e^{-a(r-r_e)}}{2}\right]\left[(\gamma+2v)e^{-a(r-r_e)}\right]^{\frac{\gamma-1}{2}} {}_1F_1\left(-v,\gamma;(\gamma+2v)e^{-a(r-r_e)}\right) \tag{6-68}$$

Note that $\gamma \geq 1$ is required to keep Eq. (6-68) from blowing up in the limit as $r \to \infty$. In addition, in order to have a square integrable eigenfunction, the requirement that $v = 0,1,2,\ldots$ is now implemented.

In order to express Eq. (6-68) such that γ does not appear in it explicitly, Eq. (6-64) is used to the derive this expression:

$$(\gamma + 2v) = \pm\frac{2\sqrt{2mD}}{\hbar a} \tag{6-69}$$

The positive root in Eq. (6-69) is taken, a choice that is made since $\gamma \geq 1$ and $v \geq 0$, and substitutions are made into Eq. (6-68), leading to the final expression for the eigenfunction:

$$u(r) = N\exp\left[-\frac{\sqrt{2mD}}{\hbar a}e^{-a(r-r_e)}\right]\left[\frac{2\sqrt{2mD}}{\hbar a}e^{-a(r-r_e)}\right]^{\frac{\sqrt{2mD}}{\hbar a}-\left(v+\frac{1}{2}\right)}$$

$$\times {}_1F_1\left(-v,\frac{2\sqrt{2mD}}{\hbar a}-2v;\frac{2\sqrt{2mD}}{\hbar a}e^{-a(r-r_e)}\right) \tag{6-70}$$

An expression for γ, derived from Equation (6-69), can also be used to rewrite the now quantized energy, Eq. (6-66), as

$$E=\frac{\hbar^2a^2}{2m}\left(\nu+\frac{1}{2}\right)\left(\frac{2\sqrt{2mD}}{\hbar a}-\nu-\frac{1}{2}\right) \tag{6-71}$$

6-5 Summary. In this chapter, the confluent hypergeometric equation, transformed into Eq. (6-8), has been matched with the radial Schrödinger equation. The purpose was to demonstrate the method of matching of the constants as a method of deriving exactly solvable potentials. The conditions on G that led to deriving the Coulomb, harmonic oscillator, and Morse $\ell=0$ potentials are given in Table 6-1 along with G, and the potential and energy derived from the given G.

A very important result of this chapter is Eq. (6-8). It is important because, as mentioned above, other conditions on G, different from the three listed in this chapter, may lead to new exactly solvable potentials in later research. In addition, Eq. (6-8) will be used again in Chapter 8 where it is matched with the radial Klein-Gordon.

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{G'^2}{G^2}+\left(\frac{\gamma}{2}+\nu\right)\frac{G'^2}{G}-\frac{1}{4}G'^2\right]\frac{e^{-G/2}G^{\gamma/2}}{\sqrt{|G'|}}\,{}_1F_1(-\nu,\gamma;G)=0$$

TABLE 6-1

	$G'^2=$constant	$\frac{G'^2}{G}=$constant	$\frac{G'^2}{G^2}=$constant
$G(r)$	c_1r	Ar^2	Ae^{-ar}
$V(r)$	$\frac{-e^2}{r}$	$\frac{1}{2}m\omega^2r^2$	$D\left\{e^{-a(r-r_e)}-1\right\}^2$
E	$\frac{-me^4}{2\hbar^2n^2}$	$\hbar\omega\left(n+\frac{3}{2}\right)$	$\frac{\hbar^2a^2}{2m}\left(\nu+\frac{1}{2}\right)\left(\frac{2\sqrt{2mD}}{\hbar a}-\nu-\frac{1}{2}\right)$

CHAPTER 7

HYPERGEOMETRIC EQUATION

The method of matching the constants is used to match the radial Schrödinger equation with the hypergeometric differential equation (HGDE). Three exactly solvable potentials are derived, the Wood-Saxon, Pöschl-Teller, and Hulthén potentials.

7-1 Preliminary algebra with the hypergeometric differential equation. The hypergeometric equation is

$$x(1-x)y''(x)+\left[c-(a+b+1)x\right]y'(x)-aby(x)=0 \tag{7-1}$$

$$y(x)={}_2F_1(a,b;c;x)$$

$$=1+\frac{a\cdot b}{c}\frac{x}{1!}+\frac{a(a+1)b(b+1)}{c(c+1)}\frac{x^2}{2!}+\ldots \tag{7-3}$$

In Eq. (7-2), note that a and b are interchangeable, such that ${}_2F_1(a,b;c;x)={}_2F_1(b,a;c;x)$, and that the infinite series is truncated for a or $b=0,1,2,\ldots$. Furthermore, $c=0,1,2,\ldots$ is to be avoided.

From the outset, rather than waiting to make this switch until a later step in the algebra like we did in Chapter 6, $G(r)$ replaces x in Eq. (7-1), and using the shorthand notation introduced in Chapter 5, the HGDE is written as

$$\left[G(1-G),c-(a+b+1)G,-ab\right]\ y(G)=0 \tag{7-3}$$

Standard form of Eq. (7-3) is

$$\left[1,\frac{c-(a+b+1)G}{G(1-G)},\frac{-ab}{G(1-G)}\right]\ y(G)=0 \tag{7-4}$$

From standard form, an equation that is in invariant form is obtained. A substitution is needed for $y(G)$, and according to Eq. (5-4), this substitution is

$$y(G) = \exp\left[\tfrac{-1}{2}\int \frac{c-(a+b+1)G}{G(1-G)}\,dG\right]\psi(G) \tag{7-5}$$

The integral can be found using the method of partial fractions. Equation (7-5) is then solved for $\psi(G)$, in terms of $y(G)$, to find that

$$\psi(G) = |G|^{c/2}\,|1-G|^{\frac{(a+b+1)-c}{2}}\,{}_2F_1(a,b;c;G) \tag{7-6}$$

Equation (7-6) is the solution to the differential equation that is in invariant form. Note the replacement of ${}_2F_1(a,b;c;G)$ for $y(G)$ in going from Eq. (7-5) to Eq. (7-6).

The invariant function of the differential equation we seek is found by substituting $\tilde{F}_0 = \dfrac{-ab}{G(1-G)}$ and $\tilde{F}_1 = \dfrac{c-(a+b+1)G}{G(1-G)}$ into Eq. (5-6). After one differentiation and some algebra, this invariant function can be written as

$$I(G) = \frac{c(2-c)}{4G^2(1-G)^2} + \frac{2c(a+b-1)-4ab}{4G(1-G)^2} + \frac{1-(a-b)^2}{4(1-G)^2} \tag{7-7}$$

Having the invariant function, Eq. (7-7), and the solution, Eq. (7-6), the HGDE transformed to an equation in invariant form is

$$\left[1,0,\frac{c(2-c)}{4G^2(1-G)^2} + \frac{2c(a+b-1)-4ab}{4G(1-G)^2} + \frac{1-(a-b)^2}{4(1-G)^2}\right]$$

$$\times |G|^{c/2}\,|1-G|^{\frac{a+b+1-c}{2}}\,{}_2F_1(a,b;c;G) = 0 \tag{7-8}$$

A switch in variables from $G(r)$ to r is now made. Equation (5-23) gives the end result of such a switch. Applying Eq. (5-23), using the invariant function and solution of Eq. (7-8), the following equation is derived:

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+\frac{c(2-c)G'^2}{4G^2(1-G)^2}+\frac{[c(a+b-1)-2ab]G'^2}{2G(1-G)^2}+\frac{[1-(a-b)^2]G'^2}{4(1-G)^2}\right]$$
$$\times\frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G)=0 \qquad (7\text{-}9)$$

Equation (7-9) is important because it is a *solved* equation. What we seek in this equation is G, which is to be determined by the need of wanting a constant term in the invariant function. The successful outcome of matching Eq. (7-9), for a given G, with the radial Schrödinger or Klein-Gordon equation, is a derived potential and energy, and a specific eigenfunction whose form we already have.

Three separate conditions on G that lead to a constant term in the invariant function of Eq. (7-9) are as follows:

$$\frac{G'^2}{(1-G)^2}=c_1^{\,2} \qquad (7\text{-}10)$$

$$\frac{G'^2}{G(1-G)^2}=c_1^{\,2} \qquad (7\text{-}11)$$

$$\frac{G'^2}{G^2(1-G)^2}=c_1^{\,2} \qquad (7\text{-}12)$$

In each of these equations, until otherwise specified, c_1 is an arbitrary, positive, real constant. Equation (7-10) will be subject of the next section.

7-2 Wood-Saxon potential. Solving Eq. (7-10) for G begins the process toward deriving the Wood-Saxon potential. After taking the square root of both sides of Eq. (7-10), and using $G'=dG/dr$, we find that Eq. (7-10) is equivalent to the integral

$$\int\frac{dG}{(1-G)}=\pm\int c_1\,dr \qquad (7\text{-}13)$$

Integrating both sides of Eq. (7-13) and exponentiating, leads to

$$\left|\frac{1}{1-G}\right| = e^{\pm c_1 r + c_2} \tag{7-14}$$

In dropping the absolute value sign, our choice is to take the denominator of Eq. (7-14) as $G-1$. Furthermore, in the exponential, the negative sign will be kept over the positive sign. These choices are made because they lead to the derivation of the Wood-Saxon potential.

With the above choices in mind, G is algebraically derived form Eq. (7-14) as

$$G = 1 + e^{c_1 r - c_2} \tag{7-15}$$

Substituting the appropriate derivatives of Eq. (7-15) back into Eq. (7-9), which is rewritten below for convenience,

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + \frac{c(2-c)G'^2}{4G^2(1-G)^2} + \frac{[c(a+b-1)-2ab]G'^2}{2G(1-G)^2} + \frac{\left[1-(a-b)^2\right]G'^2}{4(1-G)^2}\right]$$

$$\times \frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G) = 0 \tag{7-9}$$

leads to an invariant function of

$$I(r) = \frac{c(2-c)c_1^2}{4\left(1+e^{c_1 r - c_2}\right)^2} + \frac{[c(a+b-1)-2ab]c_1^2}{2\left(1+e^{c_1 r - c_2}\right)} - c_1^2\left(\frac{a-b}{2}\right)^2 \tag{7-16}$$

The terms of Eq. (7-16) will now be matched with the terms of the invariant function of the Schrödinger equation. The radial Schrödinger equation in invariant form is

$$\left[1,0,\frac{-\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2}V(r) + \frac{2m}{\hbar^2}E\right]u(r) = 0 \tag{5-10}$$

As the matching begins, we set $\ell = 0$, and equate

$$\frac{2m}{\hbar^2}E = -c_1^2\left(\frac{a-b}{2}\right)^2 \tag{7-17}$$

$$\frac{-2m}{\hbar^2}V(r) = \frac{c(2-c)c_1^2}{4\left(1+e^{c_1 r - c_2}\right)^2} + \frac{\left[c(a+b-1)-2ab\right]c_1^2}{2\left(1+e^{c_1 r - c_2}\right)} \tag{7-18}$$

We set $c = 2$ in Eq. (7-18) (observing that $c = 0$ is not an option because that choice would cause Eq. (7-2) to blow up) and solve for $V(r)$, which gives

$$V(r) = -\left(\frac{\hbar^2}{2m}(a+b-1-ab)c_1^2\right)\frac{1}{1+e^{c_1 r - c_2}} \tag{7-19}$$

In order to compare Eq. (7-19) with the Wood-Saxon potential, as given in Flügge (1971, p. 162), the following definitions are made:

$$V_0 = \frac{\hbar}{2m}\frac{(a+b-1-ab)}{\overline{a}^2} \tag{7-20a}$$

$$c_1 = \frac{1}{\overline{a}} \tag{7-20b}$$

$$c_2 = \frac{R}{\overline{a}} \tag{7-20c}$$

The constants $\overline{a}$ and R are introduced to coincide with the physical parameters a and R found in Flügge (1971, p. 162). Equation (7-19) now becomes

$$V(r) = \frac{V_0}{1+e^{\frac{r-R}{\overline{a}}}} \tag{7-21}$$

With the Wood-Saxon potential derived by means of matching of the constants, an expression for the energy is also found. Using the definition for c_1, given in Eq. (7-20b), and some algebra, Eq. (7-17) becomes

$$E = -\frac{\hbar^2}{2m}\left(\frac{1}{\overline{a}^2}\right)\left(\frac{a-b}{2}\right)^2 \tag{7-22}$$

Quantization of the energy is yet to be established as attention is now turned to the eigenfunction.

The unnormalized eigenfunction, in its most general terms, can simply be read off from Eq. (7-9) as

$$u(r)=\frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G) \tag{7-23}$$

Putting Eq. (7-23) into a form that is comparable with Flügge (1971, p. 163) requires the application of the following relationship:

$${}_2F_1(a,b;c;G)=\frac{\Gamma(c)\Gamma(b-a)}{\Gamma(b)\Gamma(c-a)}(-G)^{-a}\,{}_2F_1\left(a,1-c+a;1-b+a;\frac{1}{G}\right)$$

$$+\frac{\Gamma(c)\Gamma(a-b)}{\Gamma(a)\Gamma(c-b)}(-G)^{-b}\,{}_2F_1\left(b,1-c+b;1-a+b;\frac{1}{G}\right) \tag{7-24}$$

(Abramowitz, 1972, p. 559). Using $G=1+e^{(r-R)/\bar{a}}$, recalling that $c=2$, and with the definitions

$$\nu=\frac{a-b}{2},\ \text{and}\ \mu=\frac{a+b}{2}-1 \tag{7-25}$$

it is an algebraic exercise to write the unnormalized solution as

$$u(r)=A\left(\frac{1}{1+e^{\frac{r-R}{\bar{a}}}}\right)^{\nu}\left(\frac{e^{\frac{r-R}{\bar{a}}}}{1+e^{\frac{r-R}{\bar{a}}}}\right)^{\mu}{}_2F_1\left(\mu+\nu,\mu+\nu+1;2\nu+1;\frac{1}{1+e^{\frac{r-R}{\bar{a}}}}\right)$$

$$+B\left(\frac{1}{1+e^{\frac{r-R}{\bar{a}}}}\right)^{-\nu}\left(\frac{e^{\frac{r-R}{\bar{a}}}}{1+e^{\frac{r-R}{\bar{a}}}}\right)^{\mu}{}_2F_1\left(\mu-\nu,\mu-\nu+1;1-2\nu;\frac{1}{1+e^{\frac{r-R}{\bar{a}}}}\right) \tag{7-26}$$

where A and B are constants. The second solution, with a $-\nu$ instead of a $+\nu$, is rejected if $r \to \infty$ is a boundary condition.

Quantization of energy is *not* established by taking $\mu + \nu$ or $\mu + \nu + 1 = -n$, $n = 0,1,2,\ldots$. Doing so would be incorrect because μ is imaginary. To see this, Eqs. (7-22) and (7-20a) are rewritten in terms of ν and μ, such that

$$\frac{2mE}{\hbar^2}\bar{a} = -\nu^2 \tag{7-27}$$

$$\frac{2mV_0}{\hbar^2}\bar{a} = \nu^2 - \mu^2 \tag{7-28}$$

Next, Eqs. (7-27) and (7-28) are added together, leading to

$$\frac{2m\bar{a}}{\hbar^2}(E + V_0) = -\mu^2 \tag{7-29}$$

Finally, since the left-hand side of the above equation is positive, μ must be strictly imaginary. A transcendental equation which ultimately relates E and V_0, found in Flügge (1971, p. 165), will not be pursued here.

7-3 Pöschl-Teller potential. The next potential to be derived with the method of matching of the constants is the Pöschl-Teller potential. To begin, recall Eq. (7-11):

$$\frac{G'^2}{G(1-G)^2} = c_1^{\,2} \tag{7-11}$$

This equation is square rooted prior to integrating, leading to

$$\int \frac{dG}{\sqrt{G}(1-G)} = \int \pm c_1\, dr \tag{7-30}$$

The integral on the left hand side of the equation was found using the software *Mathematica*. It can also be found in Gradshteyn (1980, p. 71). After integration and exponentiating, Eq. (7-30) becomes

$$\left|\frac{1+\sqrt{G}}{1-\sqrt{G}}\right| = e^{\pm c_1 r + c_2} \tag{7-31}$$

In dropping the absolute value signs, the right-hand side of this equation could be taken to be positive or negative. We choose to take the positive. An additional choice is made such that the constant of integration c_2 is equal to zero. Furthermore, by defining $\alpha \equiv \pm c_1$, the choice between $+c_1$ and $-c_1$ is deferred until later. Solving for G now leads to

$$G = \left[\frac{e^{\alpha r}-1}{e^{\alpha r}+1}\right]^2 = \tanh^2\left(\alpha r/2\right) \tag{7-32}$$

Higher derivatives of Eq. (7-32) are taken and substitutions are made into Eq. (7-9):

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+\frac{c(2-c)G'^2}{4G^2(1-G)^2}+\frac{\left[c(a+b-1)-2ab\right]G'^2}{2G(1-G)^2}+\frac{\left[1-(a-b)^2\right]G'^2}{4(1-G)^2}\right]$$

$$\times \frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G) = 0 \tag{7-9}$$

After the use of standard identities and algebra, we obtain an invariant function of

$$I(r) = \frac{\alpha^2}{4}\left[\frac{-(c-\frac{1}{2})(c-\frac{3}{2})}{\sinh^2(\alpha r/2)}+\frac{(a-b+\frac{1}{2})(a-b-\frac{1}{2})}{\cosh^2(\alpha r/2)}\right]-\frac{\alpha^2}{4}(a+b-c)^2$$

This equation will be referred to as Eq. (7-33). At this point, a choice is made to take $\alpha = +c_1 = 2i\overline{\alpha}$, and Eq. (7-33) promptly becomes

$$I(r) = -\overline{\alpha}^2\left[\frac{(c-\frac{1}{2})(c-\frac{3}{2})}{\sin^2(\overline{\alpha}r)}+\frac{(a-b+\frac{1}{2})(a-b-\frac{1}{2})}{\cos^2(\overline{\alpha}r)}\right]+\overline{\alpha}^2(a+b-c)^2 \tag{7-34}$$

In comparing Eq. (7-34) with the invariant function of the Schrödinger equation,

$$\left[1,0,\frac{-\ell(\ell+1)}{r^2}-\frac{2m}{\hbar^2}V(r)+\frac{2m}{\hbar^2}E\right]u(r) = 0 \tag{5-10}$$

we see the necessity of choosing $\ell = 0$, and in matching the remaining terms such that

$$V(r) = \frac{1}{2}\left(\frac{\hbar^2\overline{\alpha}^2}{m}\right)\left[\frac{(c-\frac{1}{2})(c-\frac{3}{2})}{\sin^2(\overline{\alpha}r)} + \frac{(a-b+\frac{1}{2})(a-b-\frac{1}{2})}{\cos^2(\overline{\alpha}r)}\right] \tag{7-35}$$

$$E = \frac{1}{2}\left(\frac{\hbar^2\overline{\alpha}^2}{m}\right)(a+b-c)^2 \tag{7-36}$$

In Eq. (7-35), the Pöschl-Teller potential is derived. Quantization of Eq. (7-36) will be seen in the following paragraphs.

Specifying the eigenfunction begins, as it did in the last section, with the following equation:

$$u(r) = \frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G) \tag{7-23}$$

With $\alpha = 2i\overline{\alpha}$ substituted into Eq. (7-32), we find that $G = -\tan^2(\overline{\alpha}r)$, which in turn is substituted into Eq. (7-23). With the use of an identity found in Abramowitz (1972, p. 559), we find

$${}_2F_1(a,b;c;G) = (1-G)^{-a}\,{}_2F_1\left(a,c-b;c;\frac{G}{G-1}\right) \tag{7-37}$$

Eq. (7-23) now becomes

$$u(r) = N(\sin\overline{\alpha}r)^{c-\frac{1}{2}}(\cos\overline{\alpha}r)^{a-b+\frac{1}{2}}\,{}_2F_1\left(a,c-b;c;\sin^2\overline{\alpha}r\right) \tag{7-38}$$

N, a normalization constant, has been introduced.

In order to cut the series in the hypergeometric function, and find quantization of energy, we define $c-b = -n(n = 0,1,2,\ldots)$. Two additional definitions are made for convenience, $c - 1/2 \equiv \chi$ and $a - b + 1/2 \equiv \lambda$. Equation (7-38), using the definitions, becomes

$$u(r) = N(\sin\overline{\alpha}r)^{\chi}(\cos\overline{\alpha}r)^{\lambda}\,{}_2F_1\left(-n,\chi+\lambda+n;\chi+\tfrac{1}{2};\sin^2\overline{\alpha}r\right) \tag{7-39}$$

Furthermore, the potential and energy are rewritten as

$$V(r)=\frac{1}{2}\left(\frac{\hbar^2\overline{\alpha}^2}{m}\right)\left[\frac{\chi(\chi-1)}{\sin^2\overline{\alpha}r}+\frac{\lambda(\lambda-1)}{\cos^2\overline{\alpha}r}\right] \tag{7-40}$$

$$E=\frac{1}{2}\left(\frac{\hbar^2\overline{\alpha}^2}{m}\right)(\chi+\lambda+2n)^2 \tag{7-41}$$

Further discussion of the Pöschl-Teller potential is found in Flügge (1971, pp. 89-93), including a restriction on χ and λ, such that $\chi>1$ and $\lambda>1$. In fact, to be more in keeping with Flügge (1971), after setting $\ell=0$ at the beginning of the matching process, we would treat the problem as strictly one dimensional, replacing r with x as the independent variable, and then, in Eqs. (7-40) and (7-41), define $V_0=\hbar^2\overline{\alpha}^2/m$. A restriction is placed on x in Eq. (7-40), such that $0\le\overline{\alpha}x\le\pi/2$.

7-4 Hulthén potential. The final condition on G that is to be studied in this chapter is

$$\frac{G'^2}{G^2(1-G)^2}=c_1^{\,2} \tag{7-12}$$

After taking the square root of both sides, Eq. (7-12) is equivalent to the following:

$$\int\frac{dG}{G(1-G)}=\pm\int c_1\,dr \tag{7-42}$$

The integral on the left-hand side can be found using partial fractions. The end result of integrating both sides and exponentiating is

$$\left|\frac{G}{1-G}\right|=e^{\pm c_1 r+c_2} \tag{7-43}$$

In dropping the absolute value signs, some choices are made before solving for G. These choices are to reverse the denominator of Eq. (7-43) to $G-1$, to take $c_2=0$ and, with $c_1>0$, to keep the negative sign over the positive. Equation (7-43) then becomes

$$\frac{G}{G-1} = e^{-c_1 r} \tag{7-44}$$

Upon solving Eq. (7-44) for G, we have

$$G = \frac{-e^{-c_1 r}}{1-e^{-c_1 r}} \tag{7-45}$$

Having an expression for G, the invariant function in Eq. (7-9),

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + \frac{c(2-c)G'^2}{4G^2(1-G)^2} + \frac{[c(a+b-1)-2ab]G'^2}{2G(1-G)^2} + \frac{\left[1-(a-b)^2\right]G'^2}{4(1-G)^2}\right]$$

$$\times \frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G) = 0 \tag{7-9}$$

can now be calculated. It is easier in computing derivatives to use $G = 1/\left(1-e^{c_1 r}\right)$ and the following result reflects this rewriting of Eq. (7-45):

$$I(r) = \frac{-c_1^{\,2}}{4}(c-1)^2 + \frac{c_1^{\,2}}{4}\frac{[2c(a+b-1)-4ab]}{\left(1-e^{c_1 r}\right)} + \frac{c_1^{\,2}}{4}\frac{\left[1-(a-b)^2\right]}{\left(1-e^{c_1 r}\right)^2} \tag{7-46}$$

In comparing Eq. (7-46) with the invariant function of the Schrödinger equation,

$$\left[1,0,\frac{-\ell(\ell+1)}{r^2} - \frac{2m}{\hbar^2}V(r) + \frac{2m}{\hbar^2}E\right]u(r) = 0 \tag{5-10}$$

we again see the necessity of choosing $\ell = 0$. Furthermore, if we take $a-b = \pm 1$, killing the term on the end of Eq. (7-46), then the remaining two terms of that equation match the remaining two terms of Eq. (5-10) to give the potential energy and total energy as

$$V(r) = \left(\frac{\hbar^2}{2m}\right)\frac{c_1^{\,2}}{4}[2c(a+b-1)-4ab]\frac{e^{-c_1 r}}{1-e^{-c_1 r}} \tag{7-47}$$

$$E = \frac{-\hbar^2}{2m} c_1^2 \left(\frac{c-1}{2} \right)^2 \tag{7-48}$$

In Eq. (7-47), the Hulthén potential is derived. Quantization of energy remains to be seen.

The unnormalized eigenfunction once again begins with the equation

$$u(r) = \frac{|G|^{c/2} |1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}} {}_2F_1(a,b;c;G) \tag{7-23}$$

In conjunction with the following identity found in Abramowitz (1972, p. 559),

$${}_2F_1(a,b;c;G) = (1-G)^{-a} {}_2F_1\left(a, c-b; c; \frac{G}{G-1} \right) \tag{7-49}$$

and using $G = 1/\left(1 - e^{c_1 r}\right)$, Eq. (7-23) becomes

$$u(r) = \left(e^{-c_1 r}\right)^{\frac{c-1}{2}} \left(1 - e^{-c_1 r}\right)^{\frac{1+a-b}{2}} {}_2F_1\left(a, c-b; c; e^{-c_1 r}\right) \tag{7-50}$$

In order to truncate the hypergeometric function of Eq. (7-50) into a polynomial, the following condition is imposed: $a = 1 - n (n = 1,2,3,\ldots)$. Making a choice to take $a - b = 1$, and defining $\alpha = (c-1)/2$, Eq. (7-50) now becomes

$$u(r) = e^{-\alpha c_1 r}\left(1 - e^{-c_1 r}\right) {}_2F_1\left(2\alpha + 1 + n, 1 - n; 2\alpha + 1; e^{-c_1 r}\right) \tag{7-51}$$

Equations (7-47) and (7-48) are examined in terms of n and α in order to show quantization of energy. In so doing, we now have

$$V(r) = -V_0 \frac{e^{-c_1 r}}{1 - e^{-c_1 r}} \tag{7-52a}$$

with

$$V_0 = \left(\frac{\hbar^2}{2m} \right) c_1^2 \beta^2 \tag{7-52b}$$

such that $\beta^2 = 2c(a+b-1) - 4ab = n^2 + 2\alpha n$. The energy, now in terms of V_0, n and β^2, is

$$E = -V_0 \left(\frac{\beta^2 - n^2}{2\beta n} \right)^2 \tag{7-53}$$

Further reading on the Hulthén potential is found in Flügge (1971, pp. 175-8).

7-5 Summary. In this chapter, the hypergeometric equation, transformed into Eq. (7-9), has been matched with the radial Schrödinger equation. The purpose was to demonstrate the method of matching of the constants as a method of deriving exactly solvable potentials. The conditions on G that led us to the Wood-Saxon, Pöschl-Teller, and Hulthén potentials are given in Table 7-1, in addition to the potential and energy derived from the given G.

The important result of this chapter is Eq. (7-9), and thus it is rewritten below for emphasis. This equation is important because different choices of G, other than the three listed in this chapter, may lead to new exactly solvable potentials. In addition, Eq. (7-9) matched with the radial Klein-Gordon equation remains to be studied, and is the subject of the next chapter.

$$\left[1, 0, \frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + \frac{c(2-c)G'^2}{4G^2(1-G)^2} + \frac{[c(a+b-1)-2ab]G'^2}{2G(1-G)^2} + \frac{[1-(a-b)^2]G'^2}{4(1-G)^2} \right]$$

$$\times \frac{|G|^{s/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}} \, {}_2F_1(a,b;c;G) = 0 \tag{7-9}$$

Table 7-1 is found on the following page.

TABLE 7-1

	$\frac{G'^2}{(1-G)^2}$ =constant	$\frac{G'^2}{G(1-G)^2}$ =constant	$\frac{G'^2}{G^2(1-G)^2}$ =constant
$G(r)$	$1+e^{c_1 r-c_2}$	$-\tan(\overline{\alpha}x)$	$\frac{-e^{c_1 r}}{1-e^{c_1 r}}$
$V(r)$	$\frac{-V_0}{1+e^{\frac{r-R}{\overline{a}}}}$	$\frac{1}{2}V_0\left\{\frac{\chi(\chi-1)}{\sin^2\overline{\alpha}x}+\frac{\lambda(\lambda-1)}{\cos^2\overline{\alpha}x}\right\}$	$-V_0\frac{e^{c_1 r}}{1-e^{c_1 r}}$
E	$\frac{-\hbar^2}{2m}c_1^2\left(\frac{a-b}{2}\right)^2$	$\frac{1}{2}\left(\frac{\hbar^2\overline{\alpha}^2}{m}\right)(\chi+\lambda+2n)^2$	$-V_0\left(\frac{\beta^2-n^2}{2\beta n}\right)$

CHAPTER 8

RADIAL KLEIN-GORDON APPLICATIONS

Three exactly solvable potentials are found for the radial Klein-Gordon equation. Two of the potentials derived here are the Wood-Saxon and the Hulthén potentials, both of which were first discussed in Chapter 7 in association with the hypergeometric equation and the radial Schrödinger equation. Also, the two topics of this thesis, pertaining to strongly coupled positronium and matching of the constants, especially overlap in deriving the third potential, the Coulomb potential.

8-1 The hypergeometric and Klein-Gordon equations. In the first section of Chapter 7, the following equation was derived:

$$\left[1,0,\frac{1}{2}\frac{G'''}{G'}-\frac{3}{4}\frac{G''^2}{G'^2}+\frac{c(2-c)G'^2}{4G^2(1-G)^2}+\frac{[c(a+b-1)-2ab]G'^2}{2G(1-G)^2}+\frac{[1-(a-b)^2]G'^2}{4(1-G)^2}\right]$$

$$\times\frac{|G|^{c/2}|1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}}\,{}_2F_1(a,b;c;G)=0 \tag{7-8}$$

This equation is important because it is the working equation in finding exactly solvable potentials with hypergeometric functions as solutions, in using the method of matching of the constants. In fact, three exactly solvable potentials were found in Chapter 7 for the radial Schrödinger equation, one for each of the following three conditions on G:

$$\frac{G'^2}{(1-G)^2}=c_1^{\,2} \tag{7-10}$$

$$\frac{G'^2}{G(1-G)^2}=c_1^{\,2} \tag{7-11}$$

$$\frac{G'^2}{G^2(1-G)^2}=c_1^{\,2} \tag{7-12}$$

where c_1 represents an arbitrary constant.

In the first two sections of this chapter, Eq. (7-10) followed by Eq. (7-12) are used to determine the function $G(r)$, enabling matching of the constants to take place between the radial Klein-Gordon:

$$\left[1,0,V(r)^2 - 2EV(r) - \frac{\ell(\ell+1)}{r^2} - \left(m^2 - E^2\right)\right]u(r) = 0 \tag{8-1}$$

and Eq. (7-8). We note the use of natural units in Eq. (8-1), and that although this equation was first encountered as Eq. (2-9), it is written here in the shorthand notation of Chapter 5.

8-2 Wood-Saxon potential. The condition on G given above in Eq. (7-10), is satisfied for

$$G = 1 + e^{c_1 r - c_2} \tag{8-2}$$

where c_1 and c_2 unspecified constants. The required derivatives of Eq. (8-2) are taken and after substitution, the invariant function of Eq. (7-8) becomes

$$I = \frac{c(2-c)c_1^2}{4\left(1+e^{c_1 r - c_2}\right)^2} + \frac{\left[c(a+b-1)-2ab\right]c_1^2}{2\left(1+e^{c_1 r - c_2}\right)} - c_1^2\left(\frac{a-b}{2}\right)^2 \tag{8-3}$$

The following definitions are made for convenience:

$$x = 1 + e^{c_1 r - c_2} \tag{8-4a}$$

$$\alpha = \frac{c(2-c)}{4} \tag{8-4b}$$

$$\beta = \frac{c(a+b-1)-2ab}{2} \tag{8-4c}$$

$$\delta = \left(\frac{a-b}{2}\right)^2 \tag{8-4d}$$

such that Eq. (8-3) can be written in a more compact way:

$$I = \frac{c_1^2 \alpha}{x^2} + \frac{c_1^2 \beta}{x} - c_1^2 \delta \tag{8-5}$$

The terms of Eq. (8-5) are now matched with the invariant function of the radial Klein-Gordon equation.

The radial Klein-Gordon equation, written again here for easy reference, is

$$\left[1, 0, V(r)^2 - 2EV(r) - \frac{\ell(\ell+1)}{r^2} - \left(m^2 - E^2\right)\right] u(r) = 0 \tag{8-1}$$

We set $\ell = 0$ and match terms with Eq. (8-5) in the following ways:

$$V^2 = \frac{c_1^2 \alpha}{x^2} \tag{8-6}$$

$$-2EV = \frac{c_1^2 \beta}{x} \tag{8-7}$$

$$-\left(m^2 - E^2\right) = -c_1^2 \delta \tag{8-8}$$

Defining a separation constant as k, Eq. (8-7) can be rearranged such that

$$-xV = k = \frac{c_1^2 \beta}{2E} \tag{8-9}$$

Solving the equality on the left in Eq. (8-9) for the potential, leads to

$$V(r) = \frac{-k}{x} = \frac{-k}{1 + e^{c_1 r - c_2}} \tag{8-10}$$

Furthermore, comparing Eq. (8-10) with Eq. (8-6) implies that $k^2 = c_1^2 \alpha$, allowing Eq. (8-10) to be written in terms of the constant c_1, and the hypergeometric function parameter, c

with the help of Eq. (8-4b). Either way, Eq. (8-10) is of the same form as the Wood-Saxon potential given in Eq. (7-21).

Having derived the potential, an expression for the energy is found. From the right-hand equality in Eq. (8-9), we find that

$$E = \frac{c_1^2 \beta}{2k} \tag{8-11}$$

Squaring both sides of Eq. (8-11), followed by the substitutions $k^2 = c_1^2 \alpha$ and $c_1^2 = \left(m^2 - E^2\right)/\delta$, this latter expression having been derived from Eq. (8-8), leads to expressing the energy as

$$E^2 = \frac{m^2}{1 + \dfrac{4\alpha\delta}{\beta^2}} \tag{8-12}$$

In terms of the defining parameters of the hypergeometric function, we have

$$E^2 = \frac{m^2}{1 + \dfrac{c(2-c)(a-b)^2}{\left[c(a+b-1) - 2ab\right]^2}} \tag{8-13}$$

Quantization of energy, as we have seen, comes from imposing square integrability on the solution, which is in the general form of Eq. (7-23):

$$u(r) = \frac{|G|^{c/2} |1-G|^{\frac{a+b+1-c}{2}}}{\sqrt{|G'|}} \, {}_2F_1(a,b;c;G) \tag{7-23}$$

The problem will not be pursued beyond this point, but the physical solution is needed, however, if the Wood-Saxon potential were to be used as a truncating potential of the Coulomb potential.

8-3 Hulthén potential. The second condition on G that is examined, is

$$\frac{G'^2}{G^2(1-G)^2} = c_1^{\,2} \tag{7-12}$$

In Sec. 7-4 of Chapter 7, it was shown that Eq. (7-12) is satisfied for

$$G = \frac{-e^{-c_1 r}}{1-e^{-c_1 r}} \tag{7-45}$$

From Eq. (7-45), the invariant function in Eq. (7-8), an equation also given at the beginning of this chapter, can now be calculated. In practice, it was easier in computing derivatives to rewrite Eq. (7-45) as $G = 1/\left(1-e^{c_1 r}\right)$. The resulting invariant function is

$$I(r) = \frac{-c_1^{\,2}}{4}(c-1)^2 + \frac{c_1^{\,2}}{4}\frac{[2c(a+b-1)-4ab-1]}{\left(1-e^{c_1 r}\right)} + \frac{c_1^{\,2}}{4}\frac{\left[1-(a-b)^2\right]}{\left(1-e^{c_1 r}\right)^2} \tag{8-14a}$$

$$= \frac{c_1^2\alpha}{x^2} + \frac{c_1^2\beta}{x} - c_1^2\delta \tag{8-14b}$$

where

$$x = 1-e^{c_1 r} \tag{8-15}$$

$$\alpha = \frac{1-(a-b)^2}{4} \tag{8-16}$$

$$\beta = \frac{2c(a+b-1)-4ab-1}{4} \tag{8-17}$$

$$\delta = \frac{(c-1)^2}{4} \tag{8-18}$$

In matching terms of Eq. (8-14b) with terms of the invariant function of the radial Klein-Gordon equation,

$$\left[1,0,V(r)^2 - 2EV(r) - \frac{\ell(\ell+1)}{r^2} - \left(m^2 - E^2\right)\right]u(r) = 0 \tag{8-1}$$

the algebra of the last section can be used again by noting that the form of Eq. (8-14b) is identical to the form of Eq. (8-5). Therefore, for $\ell = 0$, the potential and energy can be written down immediately as

$$V(r) = \frac{-c_1\sqrt{\alpha}}{x} = \frac{c_1\sqrt{1-(a-b)^2}}{2}\left(\frac{e^{-c_1 r}}{1-e^{-c_1 r}}\right) \tag{8-19}$$

$$E^2 = \frac{m^2}{1+\dfrac{4\alpha\delta}{\beta^2}} = \frac{m^2}{1+\dfrac{4(c-1)^2\left[1-(a-b)^2\right]}{\left[2c(a+b-1)-4ab-1\right]}} \tag{8-20}$$

Equation (8-19) is in the form of Eq. (7-47) which, in turn, was recognized as the Hulthén potential in Chapter 7. This potential would not make a good truncating potential to the Coulomb potential in the study of strongly coupled positronium in that it also is singular at $r = 0$. Quantization of energy and the physical solution has not been found in this research.

8-4 Coulomb potential. We now set aside Eq. (7-8), the working hypergeometric equation, to be replaced by Eq. (6-8),

$$\left[1, 0, \frac{1}{2}\frac{G'''}{G'} - \frac{3}{4}\frac{G''^2}{G'^2} + \left(\frac{\gamma}{2} - \frac{\gamma^2}{4}\right)\frac{G'^2}{G^2} + \left(\frac{\gamma}{2} + \nu\right)\frac{G'^2}{G} - \frac{1}{4}G'^2\right]\frac{e^{-G/2}G^{\gamma/2}}{\sqrt{|G'|}}\,{}_1F_1(-\nu, \gamma; G) = 0$$

the working confluent hypergeometric equation. The above equation shall now be matched with the radial Klein-Gordon equation. Three particular conditions on G led to three exactly solvable potentials for the radial Schrödinger equation in Chapter 6.

In this section, the condition that G'^2 = constant is imposed, and for $G = c_1 r + c_2$, where c_1 and c_2 are constants, it is easy to verify that the condition this satisfied. A choice is now made to take the constant c_2 equal to zero and with $G = c_1 r$, the invariant function of Eq. (6-8), becomes

$$I(r) = \left(\frac{\gamma}{2} - \frac{\gamma^2}{4}\right)\frac{1}{r^2} + \left(\frac{\gamma}{2} + \nu\right)\frac{c_1}{r} - \frac{c_1^2}{4} \tag{8-21}$$

Equation (8-21) is matched with the invariant function of the Klein-Gordon equation, which is again written here for easy reference:

$$\left[1,0,V(r)^2-2EV(r)-\frac{\ell(\ell+1)}{r^2}-\left(m^2-E^2\right)\right]u(r)=0 \tag{8-2}$$

Matching of terms is made in the following ways:

$$V(r)^2-\frac{\ell(\ell+1)}{r^2}=\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{1}{r^2} \tag{8-22}$$

$$-2EV(r)=\left(\frac{\gamma}{2}+\nu\right)\frac{c_1}{r} \tag{8-23}$$

$$-\left(m^2-E^2\right)=\frac{-c_1^2}{4} \tag{8-24}$$

All three of these equations are immediately put to use. First, Eq. (8-24) is used to solve for the constant $c_1{}^2$:

$$c_1{}^2=4\left(m^2-E^2\right) \tag{8-25}$$

Next, the constants of Eq. (8-23) are all grouped together to give the following equality:

$$-rV(r)=\frac{c_1}{2E}\left(\frac{\gamma}{2}+\nu\right) \tag{8-26}$$

The right-hand side of Eq. (8-26) is constant, and therefore, the left-hand side of the equation must also be constant. In anticipation of the deriving the Coulomb potential, a separation constant is defined as $Z\alpha$, where Z is the atomic number and α reassumes its role as denoting the coupling constant. When the left-hand side of Eq. (8-26) is equated to $Z\alpha$, the potential is easily derived:

$$V(r)=\frac{-Z\alpha}{r} \tag{8-27}$$

The energy is derived by equating the right-hand side of Eq. (8-27) to $Z\alpha$. After squaring both sides of the equality, and making a substitution for $c_1{}^2$ according to Eq. (8-25), we find that

$$E^2 = \frac{m^2}{1+\dfrac{(Z\alpha)^2}{\left(\dfrac{\gamma}{2}+\nu\right)^2}} \tag{8-28}$$

Equation (8-28) is not the final equation for the energy, as γ can be derived from Eq. (8-22). Specifically, Eq. (8-27) is substituted into Eq. (8-22), leading to the quadratic equation,

$$\gamma^2 - 2\gamma + 4\left[(Z\alpha)^2 - \ell(\ell+1)^2\right] = 0 \tag{8-29}$$

The roots to this quadratic equation are

$$\gamma = 1 \pm 2\left[\left(\ell+\tfrac{1}{2}\right)^2 - (Z\alpha)^2\right]^{1/2} \tag{8-30}$$

Substituting the positive root of Eq. (8-30) back into Eq. (8-28) gives

$$E^2 = \frac{m^2}{1+\dfrac{(Z\alpha)^2}{\left(\nu-\frac{1}{2}+\left[(\ell+1/2)-(Z\alpha)^2\right]^{1/2}\right)^2}} \tag{8-31}$$

If we take the square root of Eq. (8-31), put back c^2 to have agreement in units, and also define $\nu = n-(\ell+1)$, then Eq. (8-31) is identical to the following expression from Landau (1990, p. 279):

$$E = \frac{mc^2}{\left\{1+\dfrac{(Z\alpha)^2}{\left(n-\ell-\frac{1}{2}+\left[(\ell+1/2)-(Z\alpha)^2\right]^{1/2}\right)^2}\right\}^{1/2}} \tag{8-32}$$

In Chapter 6, it was stated that $\nu = 0,1,2,\ldots$ is required in order to have square integrable solutions. Therefore, in proceeding to make the definition that $\nu = n-(\ell+1)$ in Eq. (8-31), we note that n is the principal quantum number, inasmuch as $n \geq \ell+1$ would be required. Thus, in this manner, which is due to square integrability, quantization of energy is obtained.

The remainder of this section will be used express the solution of Eq. (6-3), namely

$$u(r) = \frac{e^{-G/2} G^{\gamma/2}}{\sqrt{|G'|}} {}_1F_1(-\nu, \gamma; G) \tag{6-37}$$

in terms of Whittaker functions. The substitution of $G = c_1 r$ into Eq. (6-37) gives

$$u(r) = \frac{e^{-c_1 r/2} (c_1 r)^{\gamma/2}}{\sqrt{|c_1|}} {}_1F_1(-\nu, \gamma; c_1 r) \tag{8-33}$$

An algebraic exercise now begins by first deriving ν from Eq. (8-28) such that

$$\nu = \pm \frac{E(Z\alpha)}{\sqrt{m^2 - E^2}} - \frac{\gamma}{2} \tag{8-34}$$

The positive root is taken insure that $\nu \geq 0$, and the following definitions are made:

$$k = \frac{E(Z\alpha)}{\sqrt{m^2 - E^2}} \tag{8-35}$$

$$\mu = \sqrt{\left(\ell + \tfrac{1}{2}\right)^2 - (Z\alpha)^2} \tag{8-36}$$

Next, the substitution of Eq. (8-36) into Eq. (8-30) gives

$$\gamma = 1 \pm 2\mu \tag{8-37}$$

and the substitution of Eqs. (8-37) and (8-35) into Eq. (8-34) leads to an expression for $-\nu$ as

$$-\nu = \frac{1}{2} \pm \mu - k \tag{8-38}$$

Prior to substituting Eqs. (8-37) and (8-38) into Eq. (8-33), the expression for $u(r)$, the square root of both sides of Eq. (8-25) is taken such that

$$c_1 = \pm 2\sqrt{m^2 - E^2} \tag{8-39}$$

Keeping the positive root by requiring c_1 to be positive, and defining $K = \sqrt{m^2 - E^2}$, a final definition is made, namely

$$\rho = c_1 r = 2Kr \tag{8-40}$$

Finally, Eqs. (8-37), (8-38) and (8-40) are all substituted into Eq. (8-33), leading to

$$u(r) = \frac{e^{-\rho/2}\rho^{1\pm 2\mu}}{\sqrt{2K}} {}_1F_1\left(\tfrac{1}{2} \pm \mu - k, 1 \pm 2\mu; \rho\right) \tag{8-41}$$

As can be seen from the following formula,

$$M_{k,\mu}(\rho) = e^{-\rho/2}\rho^{1+2\mu} {}_1F_1\left(\tfrac{1}{2} + \mu - k, 1 + 2\mu; \rho\right) \tag{8-42}$$

(Abramowitz, 1972, p. 505), and ignoring the constant factor of $\sqrt{2K}$ in the denominator, Eq. (8-41) is exactly the two Whittaker functions $M_{k,\mu}(\rho)$ and $M_{k,-\mu}(\rho)$. Furthermore, a specific linear combination of $M_{k,\mu}(\rho)$ and $M_{k,-\mu}(\rho)$, namely

$$W_{k,\mu}(\rho) = \frac{\Gamma(-2\mu)}{\Gamma\left(\frac{1}{2} - \mu - k\right)} M_{k,\mu}(\rho) + \frac{\Gamma(2\mu)}{\Gamma\left(\frac{1}{2} + \mu - k\right)} M_{k,-\mu}(\rho) \tag{4-16}$$

constructs the other Whittaker function, $W_{k,\mu}(\rho)$, which is also the physical solution in the event that $r \to \infty$ is a consideration. See Eqs. (3-23) and (3-24).

8-5 Conclusions on matching of the constants. In this chapter, the two ends meet between matching of the constants as a method of deriving exactly solvable potentials and our original topic on strongly coupled positronium in the Crater and Van Alstine

formalism. The connection is officially made by setting $Z = 1$, $\ell = 0$, and by replacing E with ε_W and m with m_W in Eq. (8-1), the radial Klein-Gordon equation, leading to Eq. (2-21), the Crater and Van Alstine equation. Therefore, matching of the constants (specifically what was done in Sec. 8-4) has provided a third method of solving Eq. (2-21) for the pure Coulomb potential, inasmuch as this problem was solved first by a transformation to Kummer's equation in Chapter 3, and then by Frobenius' method in Chapter 4.

In addition, matching of the constants, based on the work of Sections 8-2 and 8-3, respectively, indicates that the Wood-Saxon potential and the Hulthén potential are exactly solvable potentials in the radial Klein-Gordon equation. Determining quantization of energy for these two potentials, however, remains as the subject of future work. If physical solutions were obtained, particularly for the Wood-Saxon potential, then this potential could serve as a truncating potential to the Coulomb potential in the strongly coupled positronium research. On the other hand, mathematical convenience would appear to have been lost and not gained in this quest for an exactly solvable potential.

CHAPTER 9

CONCLUSION

A two-particle relativistic wave equation, developed by Crater and Van Alstine (Van Alstine, 1986), has been used to study strongly coupled positronium with the purpose of obtaining this equation's prediction of stability or instability with regard to the spontaneous creation of real electron positron pairs. Stability, according to this equation, has been found for two potentials. In addition, the solution of the wave equation for one of these potentials did not yield a closed form solution using Frobenius' method to solve the equation. A method of finding exactly solvable potentials, matching of the constants, has been detailed, demonstrated and applied. This method can now be used to search for alternative potentials or potential truncations in the stability study of strongly coupled positronium.

9-1 Strongly coupled positronium. In Chapter 3, the ground state energy, in the center-of-momentum frame, of strongly coupled positronium as a function of the fine structure constant was obtained from an equation like the S-wave radial Klein-Gordon equation, using a regularized Coulomb potential. We recover the result of Bawin and Cugnon (Bawin, 1990), as represented in Fig 3-1, which indicates that this energy remains positive for increasing values of the fine structure constant, indicating stability.

To obtain this result, it was necessary to numerically solve a transcendental equation. The software package *Mathematica* was used to obtain roots to this equation. The transcendental equation was not solved, however, until an identity was found and used in which a primed Whittaker function could be written in terms of unprimed Whittaker functions, and until the secant method was used instead of Newton's method on *Mathematica*. The work done in Chapter 3 that finally lead to obtaining roots with *Mathematica* was followed once again in Chapter 4 where the change of truncating potential resulted in a different transcendental equation. Thus these sections in Chapter 3 could conceivably be useful again in solving future transcendental equations resulting from future potential choices.

In Chapter 4, a different potential was used. Specifically, a truncation of the Coulomb potential was accomplished with an r^2 potential. Frobenius' method was used to solve the

wave equation, confirming the solution for the Coulomb potential claimed in Chapter 3 where the differential equation was transformed into Kummer's equation, whose solutions are known to be the Whittaker functions. For the r^2 potential, the solutions are written as a power series in r. The solution, therefore, has an infinite number of terms, and we approximated the physical solution by keeping one, two and then three terms. For all three approximations, the ground state energy of strongly coupled positronium remained positive, indicating stability in real pair production. This prediction is consistent with that which was found using the potential of Chapter 3. On the other hand, it can be shown, see (Greiner 1990, p. 43) from which Fig. (4-4) is taken, that the Klein-Gordon equation, using the same potential of Chapter 4, has been solved and predicts *instability* with regard to pion pair creation in a strong field. Therefore, not only is the Crater and Van Alstine equation consistent with its prediction of stability for the two potentials studied here, it is also consistent in being contrary to the corresponding prediction from the Klein-Gordon equation. This consistency would certainly not weaken the trust one might place in the equation of Crater and Van Alstine as one of the many equations available in the literature used to describe relativistic two-particle systems.

9-2 Matching of the constants. Not having a closed form solution of the S-wave radial Klein-Gordon equation for the r^2 potential inspired the research in finding exactly solvable potentials using the method of matching of the constants. Three exactly solvable potentials were found for the Schrödinger equation in Chapter 6, starting the process with the confluent hypergeometric differential equation. Three more exactly solvable potentials were found in Chapter 7, this time starting the process with the hypergeometric differential equation. These six potentials were named in Beker (1993) as potentials that can be derived with the method of matching of the constants, and those two chapters provided mathematical details in the derivations. The search for exactly solvable potentials is not exhaustive in this work, however. Two equations were established: Eq. (6-8) in Chapter 6 from the confluent hypergeometric differential equation and Eq. (7-9) in Chapter 7 for the hypergeometric differential equation, both of which provide a sound starting point for looking for exactly solvable potentials by considering other conditions on G in these equations.

On the other hand, the potential $V(x) = 2V_0 \cos 2c_1 x$, derived in Chapter 5 starting from the Mathieu equation, was a potential for which Beker had not made any conjecture. This was an intriguing derivation of the research because it demonstrated that matching of the constants could uncover unexpected exactly solvable potentials. The same success could

not be repeated when working with the first three equations of Table 5-2. After transforming any one of those three equations, the constant potential was derived in matching terms with the Schrödinger equation. Deriving the constant potential is of note, but was not included here, because matching of the constants proved to be too involved to be the simplest and best way of handling the problem.

In Chapter 8, the ends meet between strongly coupled positronium research and matching of the constants because it is in this chapter that exactly solvable potentials are derived for the radial Klein-Gordon equation. The Coulomb potential was derived, providing a third opportunity to solve this problem in the course of this work. The three methods, namely transforming to Kummer's equation, Frobenius' series solution, and matching of the constants, illustrate the richness of the $1/r$ potential in quantum theory. In addition, the Wood-Saxon and Hulthén potentials of Chapter 7 were derived again as exactly solvable potentials for the Klein-Gordon equation. Further work is needed, however, with these potentials in the sense that square integrability of the solutions, and hence quantization of energy, was not explicitly pursued. It should be noted too that square integrability of solutions and quantized energy were not obtained here for the Mathieu problem of Chapter 5, or for the Wood-Saxon problem of Chapter 7, either, but with the difference that references where these potentials are solved for the Schrödinger equation were known to us and were given.

The r^2 potential of Eq. (1-5) was indeed sought as an exactly solvable potential for the radial Klein-Gordon equation using matching of the constants. Since this potential is like the harmonic oscillator potential of the Schrödinger equation, the condition on the function G in the transformed confluent hypergeometric differential equation of Eq. (6-8), that led to matching in the Schrödinger case, was followed without success in the Klein-Gordon case. Other possibilities on G were not pursued. In fact, after completing the research for this work, we found the potential of Eq. (1-5) that is used in Chapter 4, in Greiner (1990, p. 43), where it is substituted into the radial Klein-Gordon equation. The solution that is obtained by Greiner is comparable to the solution in Chapter 4; therefore, we probably were not going to find a closed form expression of the solution from the outset of research into matching of the constants.

Finally, in the topics of strongly coupled positronium and in deriving exactly solvable potentials via matching of the constants, we have been involved in two important problems in theoretical physics. The first is that of relativistic two-particle equations. The literature in this area is very important and no consensus has been reached yet. Our main contribution is the illustration of the stability of the Crater and Van Alstine two-particle

equation for a particular potential. The second topic of exactly solvable potentials in wave equations also has associated with it a large amount of literature in which there is no definitive answer. Our contribution is to have illustrated for several equations and several potentials the power of a particular method of finding exactly solvable potentials, that of matching of the constants.

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STRONGLY COUPLED POSITRONIUM: SOLUTION METHODS AND POTENTIALS

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ABSTRACT

The topics of strongly coupled positronium and matching of the constants as a method of deriving exactly solvable potentials, are subtopics of two important problems in theoretical physics. The first topic, pertaining to strongly coupled positronium, is that of relativistic two-particle equations. Our main contribution to this topic is the illustration of stability from the Crater and Van Alstine two-particle wave equation for a Coulomb potential with a homogeneously charged spherical truncating potential, with regard to spontaneous, real electron-positron pair creation. The second topic is that of finding exactly solvable potentials in wave equations. Our contribution to this topic is to have illustrated the power of a particular method, that of matching of the constants, by deriving previously known exactly solvable potentials for the radial Schrödinger and Klein-Gordon equations using this method.

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