JOURNAL OF COMPUTATIONAL PHYSICS **123,** 162–168 (1996)
ARTICLE NO. 0013

An Efficient Algorithm for Solving Coupled Schrödinger Type ODE's, Whose Potentials Include δ-Functions

SIAMAK S. GOUSHEH*

Center for Particle Physics, University of Texas at Austin, Austin, Texas 78712

Received January 12, 1994; revised April 27, 1995

I have used the shooting method to find the eigenvalues (bound state energies) of a set of strongly coupled Schrödinger type equations. I have discussed the advantages of the shooting method when the potentials include δ-functions. I have also discussed some points which are universal in these kind of problems, whose use make the algorithm much more efficient. These points include mapping the domain of the ODE into a finite one, using the asymptotic form of the solutions, best use of the normalization freedom, and converting the δ-functions into boundary conditions.

1. INTRODUCTION

In this paper I discuss a numerical method for solving an eigenvalue problem which is in the form of two strongly coupled Schrödinger type equations. The potentials for these equations contain δ-functions. The method used is based upon the shooting method [1]. I show how one can use some transformations and properties of this ODE, in order to make the problem suitable for the shooting method and make the algorithm efficient. In addition to the points mentioned above, I discuss the most effective way of correlating the corrections to the discrepancies during the iteration process, minimizing the number of unknowns using some limited analytic results, and the most effective way of initiating the search for the eigenvalues especially when the spectrum includes continuum parts as well as discrete parts. It is worth mentioning that this method works equally well whether or not there are δ-functions present. After displaying the results, I discuss them on physical grounds. Before discussing the numerical method, I would like to discuss briefly whence the problem arose. The reader who is interested only in the numerical method can skip to section two.

Over 30 years ago, Skyrme [2] conjectured that the solitonic excitations of the nonlinear σ-model (skyrmions) are to be associated with baryons, when the fields in the nonlinear σ-model are pions. Over the past two decades, much work has been done to confirm this conjecture [3, 4]. In particular Witten [4] showed that the solitons have to be quantized as fermions for an odd number of colors.

One method of calculating the baryon number of the skyrmion is the adiabatic method of Goldstone and Wilczek [5] or its modification by MacKenzie and Wilczek [6]. In the latter method, one couples the fermions (baryons) to a background pseudoscalar fields (pions). The background field then evolves from a topologically trivial configuration to a nontrivial one (a soliton). Meanwhile, by observing the energy spectrum of the fermion, one can deduce the vacuum polarization of the fermion field induced by the presence of the soliton. The vacuum polarization is believed to be the fermion number of the soliton. In a previous paper, I have used this method to find the baryon number of a skyrmion with sharply varying spatial profile in (3 + 1) dimensions [7]. The numerical method discussed here has been utilized in that paper. Also for a thoroughly analyzed example of vacuum polarization by solitons in (1 + 1) dimensions see Ref. [8]. This brings us to the Dirac equation for the fermion field $\psi(\mathbf{r}, t)$ in the presence of the background field $\theta(\mathbf{r})$.

$$H\psi = [\boldsymbol{\alpha}\cdot\mathbf{p} + \beta m(\cos\theta + i\gamma_5\boldsymbol{\tau}\cdot\hat{\mathbf{r}}\sin\theta)]\psi = E\psi, \quad (1)$$

where $\boldsymbol{\alpha}$, β, and γ_5 are the conventional Dirac matrices, m is the mass of the fermion, and $\boldsymbol{\tau}$ is the generator of the isospin rotation. ψ is an isodoublet Dirac spinor, i.e.,

$$\psi(\mathbf{r}, t) = \begin{pmatrix} P(\mathbf{r}, t) \\ N(\mathbf{r}, t) \end{pmatrix},$$

where P and N stand for proton and neutron, respectively. Note that H commutes with $\mathbf{K}$, $\mathbf{K}^2$, $\mathbf{I}^2$, $\mathbf{S}^2$ and the parity operator, where $\mathbf{K} = \mathbf{L} + \mathbf{S} + \mathbf{I}$ is the grand spin operator, $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$ is the spin operator, and $\mathbf{I} = \frac{1}{2}\boldsymbol{\tau}$ is the isospin operator. Hence the eigenstates of H are labeled by the eigenvalues of these operators.

The method employed in Ref. [7] to solve this Dirac equation is to find the eigenstates and eigenvalues of H through those of H^2. One can easily obtain

* Present address: Department of Physics, Shahid Beheshti University, Evin, Tehran 19834, Iran.

0021-9991/96 $12.00

$$H^2 = -\nabla^2 + m^2 + \frac{4m \sin\theta(r)}{3r}\beta(2\mathbf{S}\cdot\mathbf{I} - T) + 4m\beta(\mathbf{I}\cdot\hat{\mathbf{r}})(\mathbf{S}\cdot\nabla \sin\theta(r)) - 2im\beta\gamma_5\mathbf{S}\cdot\nabla\cos\theta(r), \tag{2}$$

where $T = 3(\mathbf{S}\cdot\hat{\mathbf{r}})(\mathbf{I}\cdot\hat{\mathbf{r}}) - \mathbf{S}\cdot\mathbf{I}$ is the spin–isospin tensor interaction. I choose $\theta(r)$ to be spherically symmetric and with the following radial dependence:

$$\theta(r) = \begin{cases} -\theta_0 & \text{if } r < r_0 \\ \theta_0 & \text{if } r > r_0. \end{cases}$$

This choice has two advantages. First, the last term in the above equation vanishes and the upper two and the lower two components of each of the Dirac spinors become decoupled and β simply becomes a numerical factor ($+1$ for the upper two components of the Dirac spinors and -1 for the lower two). Second, when the last term is absent, H^2 commutes with $(\mathbf{S}+\mathbf{I})^2$, in addition to commuting with the operators that commute with H. Hence the states can be decomposed into spin–isospin singlets and triplets. When the matrix elements of T are computed, one obtains

$$H^2\psi^{k,m}_{s,(-)^k} = \left[-\nabla_k^2 + m^2 - \frac{2m\sin\theta(r)}{r}\beta - 2m\sin\theta_0\beta\delta(r-r_0)\right]\psi^{k,m}_{s,(-)^k}, \tag{3}$$

$$H^2\psi^{k,m}_{t,(-)^k} = [-\nabla_k^2 + m^2 + 2m\sin\theta_0\beta\delta(r-r_0)]\psi^{k,m}_{t,(-)^k}; \quad k \geq 1, \tag{4}$$

$$H^2\psi^{k,m}_{t,(-)^{k+1}} \sim \begin{Bmatrix} H^2_{11} = -\nabla^2_{k-1} + m^2 + \frac{2m\sin\theta(r)k}{(2k+1)r}\beta + \frac{2m\sin\theta_0}{(2k+1)}\beta\delta(r-r_0) \\ H^2_{12} = H^2_{21} = -\frac{2m}{r}\beta\frac{\sqrt{k(k+1)}}{2k+1}[\sin\theta(r) - 2\sin\theta_0 r\delta(r-r_0)] \\ H^2_{22} = -\nabla^2_{k+1} + m^2 + \frac{2m\sin\theta(r)(k+1)}{(2k+1)r}\beta - \frac{2m\sin\theta_0}{2k+1}\beta\delta(r-r_0) \end{Bmatrix} \begin{pmatrix} \tilde{g}_1(r) \\ \tilde{g}_2(r) \end{pmatrix} \tag{5}$$

$$H^2\psi^0_{t,(-)^1} = \left[-\nabla_k^2 + \frac{2}{r^2} + m^2 + \frac{2m\sin\theta(r)}{r}\beta - 2m\sin\theta_0\beta\delta(r-r_0)\right]\psi^0_{t,(-)^1}, \tag{6}$$

where

$$\nabla_k^2 = \frac{1}{r}\partial_r^2 r - \frac{k(k+1)}{r^2}.$$

Equation (5) only applies to states with $k \geq 1$. The numerical method for solving the above ODE's are similar. In this paper I show how to solve for the eigenvalues of Eq. (5), since it is the most difficult one. The resulting eigenvalues for all of the above equations, including the case of constant θ, where the ODE's can be solved analytically, are shown in Ref. [7]. When θ is constant, the δ-functions are absent and Eq. (5) can be solved analytically. There are bound states only when $\beta \sin\theta_0 < 0$. Then the bound state energies are

$$E_N = \pm m\left[1 - \frac{\sin^2\theta_0}{N^2}\right]^{1/2}, \quad N > k, \tag{7}$$

where N is a positive integer playing the role of the principal quantum number as in the hydrogen atom case. The analytic form of the radial part of the ground state is

$$\psi^{k,m}_{t,(-)^{k+1}} \sim \begin{pmatrix} 1 + \frac{m\sin\theta_0 k}{(k+1)(2k+1)}r \\ -\left[\frac{m\sin\theta_0}{(2k+1)}\sqrt{k/(k+1)}\right]r \end{pmatrix} \times r^{k-1}\exp\{-[m\sin\theta_0/(k+1)]\,r\}; \tag{8}$$

From now on I concentrate on the case $\theta_0 = \pi/2$. This corresponds to a winding number one soliton. In the next section, I discuss a numerical method for obtaining eigenvalues of Eq. (5).

2. THE NUMERICAL METHOD

As mentioned before, I use the shooting method [1] in order to solve Eq. (5). Before discussing this method in some detail, I would like to discuss some transformations and analytic results which render the problem more managable. Most of these points are universal in these types of problems:

1. For the ODE under consideration, the range of the independent variable is $0 \le r \le \infty$. It is more efficient to transform r to a new variable x with the range $0 \le x \le 1$. One can implement this by a variety of smooth functions. I have chosen the following

$$x = \tanh(br) \quad \text{or} \quad r = \frac{1}{2b} \ln\left(\frac{1+x}{1-x}\right), \tag{9}$$

where b is an arbitrary stretch factor. Of course, as is the case with any such transformation, the advantage is the following. In the integration process, with constant width of steps in x, the width of the steps in r get progressively larger. Since the important part of the integration is usually concentrated at small values of r, this should help the adaptive step size control.

2. By studying the ODE close to $r = 0$ one can show that in that region the behaviour of the functions are

$$g_{1,k}(r) \sim r^k, \quad g_{2,k}(r) \sim r^{k+1}, \tag{10}$$

where $g \equiv r\tilde{g}$. Although at first sight it seems that $g_{2,k}$ should go as r^{k+2}, the strong coupling with $g_{1,k}$ reduces its exponent by one.

3. For large values of r, one can easily show that the solutions are exponentially decreasing

$$g_{1,2;k} = h_{1,2;k} \exp(-\lambda r), \quad \lambda \equiv \sqrt{m^2 - E^2}, \tag{11}$$

where $h_{1,2;k}$ are some polynomials of degrees $n_{1,2}$. Then

$$\frac{g'}{g} = \frac{h'}{h} - \lambda \to \frac{n}{r} - \lambda \to -\lambda, \quad \text{as } r \to \infty. \tag{12}$$

4. By going back to the original ODE, we know that the overall scale of the wavefunctions is arbitrary. Hence, to find the eigenvalues, the normalization is irrelevant and one can fix the value of one of the functions or their derivatives at some point in the range. For the algorithm, I choose to fix the value of one of the derivatives close to $r = \infty$ for the following reason. In these types of problems there are usually exponentially increasing solutions with the same eigenvalues as the exponentially decreasing ones and in physical applications one is usually interested in normalizable solutions (i.e., a bound state with probability 1). To obtain only the normalizable solutions, I fix the slope of one of the functions close to $r = \infty$ to be a very small number.

5. The presence of the δ-functions is the main reason why I choose the shooting method. Since all of the δ-functions appearing in Eq. (5) are at the same position r_0, the shooting method can be easily used. One can integrate (''shoot'') from the left and the right towards a fitting point. By choosing the fitting point to be the position of the δ-functions, one can implement them as boundary conditions on the slope discontinuities at the fitting point. To do this, one can integrate the ODE in the range $r_0 - \varepsilon \le r \le r_0 + \varepsilon$ as $\varepsilon \to 0$, to obtain

$$\left.\frac{dg_{1,k}}{dr}\right|_{r_0-\varepsilon}^{r_0+\varepsilon} = \frac{2m \sin\theta_0 \beta}{2k+1} g_{1,k}(r_0) + \frac{4m \sin\theta_0 \beta \sqrt{k(k+1)}}{2k+1} g_{2,k}(r_0), \tag{13}$$

$$\left.\frac{dg_{2,k}}{dr}\right|_{r_0-\varepsilon}^{r_0+\varepsilon} = -\frac{2m \sin\theta_0 \beta}{2k+1} g_{2,k}(r_0) + \frac{4m \sin\theta_0 \beta \sqrt{k(k+1)}}{2k+1} g_{1,k}(r_0). \tag{14}$$

Now I discuss the algorithm. Since the underlying principles of the shooting method are discussed fully in the Ref. [1], I discuss the method only very briefly with the emphasis on the implementation of the aforementioned modifications and analytic results. As mentioned before, the basic plan is to integrate from the left ($x = 0$) and the right ($x = 1$) towards the fitting point, which is chosen to be the position of the δ-functions (x_0). The integration is done using fifth-order Runge–Kutta steps with adaptive stepsize control. At the fitting point the mismatch between the functions and the departure of the slope discontinuities from the above conditions are used to correct the initial guess for the starting values of the functions and their derivatives. This is done by using the Newton–Raphson method. To do this, first the partial derivative matrix is replaced by its LU decomposition, and then the matrix equation is solved (I will discuss this part in more detail at the end of this section). Then one iterates this procedure until a set of specified tolerances on the mismatches of the values of the functions at the fitting point are satisfied.

It is worth mentioning that rather than the fifth-order Runge–Kutta integration algorithm used here, other more powerful and efficient integration algorithms could be used. For example, for the solution of the initial value one-dimensional Schrödinger equation, Raptis and Cash [9] have developed an exponential and Bessel fitted variable step method of order 6 for large r region and their own less tailored method [10] for small r region, which are both based on the two step formula of Cash and Raptis [11] with variable coefficients. For this problem their exponentially fitted method is more appropriate since the potentials fall off slower than $1/r^2$ and hence the Bessel fitted method is not very suitable, and for the large r region the solutions are indeed exponentially decaying. Also Simos [12] has developed a variable step P-stable method of order 6 and 8

with a phase lag of the same order. As far as the embedded Runge–Kutta method is concerned, Prince and Dormand [13] have developed formulae of order 6(5) and 8(7) and Dormand *et al.* [14] have developed formulae of order 8(6) and 12(10) which should be more efficient than the lower order formulae for higher precisions.

Since the main objective of this article is the illustration of the solution of a rather complicated problem using the shooting method and how to make the initialization and iteration procedure efficient, I have elected to use the classical fifth-order Runge–Kutta method for the integration part of the method. Now I continue describing the rest of the method.

The two coupled, second-order, eigenvalue problem ODE's can be turned into five coupled first-order ODE's by the standard methods. One defines the eigenvalue λ^2 as a new (constant) function which I have named $Y_{1,k}$. The rest of the variables are: $Y_{2,k}(x) = g_{1,k}(x)$, $Y_{3,k}(x) = (dg_{1,k}/dx)(x)$, $Y_{4,k}(x) = g_{2,k}(x)$, and $Y_{5,k}(x) = (dg_{2,k}/dx)(x)$. Then the ODE becomes

$$\begin{aligned}
\frac{dY_1}{dx} &= 0,\\
\frac{dY_2}{dx} &\equiv Y_3,\\
\frac{dY_3}{dx} &= \frac{1}{[b(1-x^2)]^2}\left\{\left[\frac{k(k-1)}{r^2} + \frac{2km\sin\theta(r)}{(2k+1)r}\beta + Y_1\right]Y_2\right.\\
&\quad \left. - \frac{2m\sqrt{k(k+1)}\sin\theta(r)}{(2k+1)r}\beta Y_4\right\} + \frac{2x}{1-x^2}Y_3,\\
\frac{dY_4}{dx} &\equiv Y_5,\\
\frac{dY_5}{dx} &= \frac{1}{[b(1-x^2)]^2}\\
&\quad \left\{\left[\frac{(k+1)(k+2)}{r^2} + \frac{2(k+1)m\sin\theta(r)}{(2k+1)r}\beta + Y_1\right]Y_4\right.\\
&\quad \left. - \frac{2m\sqrt{k(k+1)}\sin\theta(r)}{(2k+1)r}\beta Y_2\right\} + \frac{2x}{1-x^2}Y_5.
\end{aligned} \tag{15}$$

Now I discuss the boundary conditions. As is usually the case, one cannot start the integration exactly at $x = 0$ or $x = 1$, but only close to these values. The boundary conditions are $Y_2(0) = Y_4(0) = Y_2(1) = Y_4(1) = 0$, in addition to the overall scale freedom. To implement these close to the boundaries, one can choose three boundary conditions close to $x = 1$ (using the scale freedom) and two close to $x = 0$. To generate a complete starting vector $\mathbf{Y}$ close to $x = 0$ and $x = 1$, one can use an arbitrary five-component vector $\mathbf{V}$, whose first three components, along with the two boundary conditions, are used to generate the starting value of $\mathbf{Y}$ close to $x = 0$, and whose last two components, along with the three boundary conditions, are used to generate the starting value of $\mathbf{Y}$ close to $x = 1$. However, this poses an unnecessary burden on the algorithm. Since the eigenvalue $Y_{1,k}$ is constant, we can use the same value for it at $x = 0$ and $x = 1$, and since its derivative is zero, its values at the fitting point will automatically match and the matching conditions reduces to solving a 4×4 system, rather than a 5×5 one. Using this point greatly increases the radius of convergence. Using the analytic results recorded in Eqs. (10), (12), the four components of $\mathbf{V}$ are used as

$$\begin{aligned}
Y_{1,k}(\varepsilon_1) &= V_1,\\
Y_{1,k}(1-\varepsilon_2) &= V_1,
\end{aligned} \tag{16}$$

$$\begin{aligned}
Y_{2,k}(\varepsilon_1) &= \frac{\varepsilon_1}{k}V_2,\\
Y_{2,k}(1-\varepsilon_2) &= -\frac{b[1-(1-\varepsilon_2)^2]}{\sqrt{V_1}}V_4,
\end{aligned} \tag{17}$$

$$\begin{aligned}
Y_{3,k}(\varepsilon_1) &= V_2,\\
Y_{3,k}(1-\varepsilon_2) &= V_4,
\end{aligned} \tag{18}$$

$$\begin{aligned}
Y_{4,k}(\varepsilon_1) &= \frac{\varepsilon_1}{k+1}V_3,\\
Y_{4,k}(1-\varepsilon_2) &= -\frac{b[1-(1-\varepsilon_2)^2]}{\sqrt{V_1}}FIX,
\end{aligned} \tag{19}$$

$$\begin{aligned}
Y_{5,k}(\varepsilon_1) &= V_3,\\
Y_{5,k}(1-\varepsilon_2) &= FIX,
\end{aligned} \tag{20}$$

where $\varepsilon_{1,2}$ are some small numbers and *FIX* is a small fixed number corresponding to the overall scale freedom. To start the program one must supply some initial value for $\mathbf{V}$. The routine then integrates the differential equation from $x = 0$ and $x = 1$ towards the fitting point x_0. At the fitting point the matching conditions are (recall that the values of $Y_{1,k}$ from the left and right already match)

$$F_{1,k} = -Y_{2,k}\Big|_{x_0-\varepsilon}^{x_0+\varepsilon}, \tag{21}$$

$$\begin{aligned}
F_{2,k} = &-Y_{3,k}\Big|_{x_0-\varepsilon}^{x_0+\varepsilon} + \frac{1}{b(1-x_0^2)}\left[\frac{2m\sin\theta_0\beta}{2k+1}Y_{2,k}(x_0)\right.\\
&\left. + \frac{4m\sin\theta_0\beta\sqrt{k(k+1)}}{2k+1}Y_{4,k}(x_0)\right]
\end{aligned} \tag{22}$$

$$F_{3,k} = -Y_{4,k}\Big|_{x_0-\varepsilon}^{x_0+\varepsilon}, \tag{23}$$

$$F_{4,k} = -\,Y_{5,k}\Big|_{x_0-\varepsilon}^{x_0+\varepsilon} + \frac{1}{b(1-x_0^2)}\left[-\frac{2m\sin\theta_0\beta}{2k+1}\,Y_{4,k}(x_0) + \frac{4m\sin\theta_0\beta\sqrt{k(k+1)}}{2k+1}\,Y_{2,k}(x_0)\right] \tag{24}$$

Note that if there are no δ-functions present in the problem, the slopes of the functions would have to match, and the second pieces of the RHS's of Eqs. (22), (24) would be missing. For a perfect solution, the discrepancy vector **F** should vanish. After one round of integration **F** is computed. Then the routine alters each of the values of the components of **V** separately by the corresponding components of $\delta\mathbf{V}$ (initially user supplied) and repeats the integration to obtain a new set of discrepancy vectors. Then from the difference between these quantities, it computes

$$(A)_{ij} \equiv \frac{\partial F_i}{\partial V_j}.$$

Then by using A and **F**, the algorithm solves for a set of corrections to the **V**, named **B**, so as to make the discrepancy zero after the next round of integration. This is done by using Newton-Raphson method to solve for the correction **B** and then adding it to **V**,

$$(A)_{ij}B_j = -F_i, \quad \text{where } 1 \le i,j \le 4, \tag{25}$$

$$V_i^{\text{new}} = V_i + B_i, \tag{26}$$

The process continues until a desired accuracy constraint on, for example, the eigenvalue is satisfied. In practice I have found that when the initial guesses on the values of the derivatives are within a factor of 10 and that of the eigenvalue within 0.1, after about seven iterations one obtains a factor of 10^{-12} accuracy (using double precision). When I used the program for the case of constant θ, in which case I had solved the system analytically, a factor of 10^{-12} accuracy reported by the program was only accurate to 10^{-10} as compared to the actual value. This is due to the approximate nature of the implementation of Eqs. (10), (12) only close to the boundaries. Two additional points are worth mentioning:

• "Aim" the eigenvalue from above. When the program is searching for an eigenvalue, each of the eigenvalues has a certain pull or attraction. In general, I have found that the larger the absolute value of the eigenvalue (i.e., more strongly bound, in the case of bound states) the larger the pull. Even though each of the eigenvalues in the continuum should not have any pull, the whole continuum seems to have a finite pull. For this reason, when searching for an eigenvalue, it is best to set the initial guess slightly higher (away from the continuum) than its expected value even if there are no states between the state in question and the continuum. If there are states between the one in question and the continuum, of course the pull towards the lower values becomes stronger.

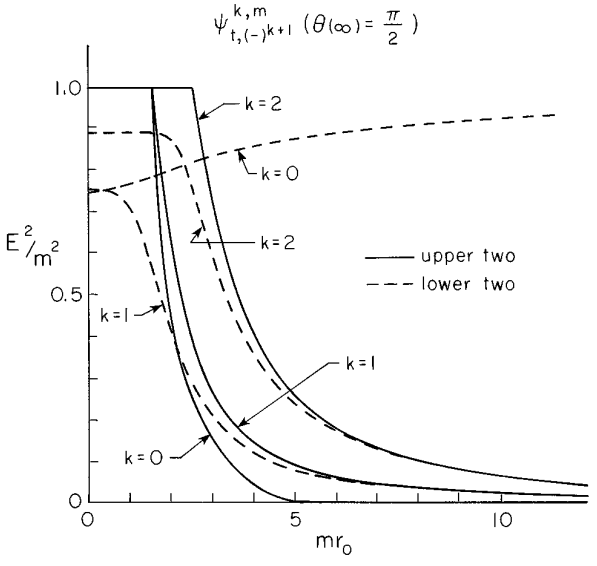

FIG. 1. The energy levels for $\psi^{k,m}_{t,(-)^{k+1}}$ as a function of mr_0 (r_0 is the position of the δ-functions), for $k = 0, 1, 2$ when $\theta_0 = \pi/2$. These states are the solutions to Eqs. (5), (6). The eigenvalues of these equations $\lambda^2 = m^2 - E^2$ were obtained by the shooting method as described in the text. The "upper and lower two" labels refer to the upper and lower two components of the Dirac spinors in the original Dirac equation (Eq. (1)) and are distinguished by the parameter $\beta = 1$ and $\beta = -1$, respectively.

• One additional point can be taken into account which helps the convergence of the iteration process. The increments $\delta\mathbf{V}$ used for the differentiation should partially depend on the correction vector **B** for the following reason. Suppose the initial value of **V** was off by a factor of 1000. Then, if the values of $\delta\mathbf{V}$ and **B** are correlated, after the next round of integrations, the subroutine using Newton–Raphson method to find the corrections for the next round, will get a more realistic information from the matrix A regarding how the necessary changes will *actually* alter **F**. This will definitely increase the radius of convergence. In the latter stages of the iteration process, where the value of **V** is more or less pinned down, one needs to know the response of **F** to smaller values of **B**. However, in practice we want $10^{-5}\mathbf{V} \le \delta\mathbf{V} \le 10^{-1}\mathbf{V}$; otherwise the derivatives become meaningless. Hence we set $\delta\mathbf{V} \equiv \mathbf{B}$, but subject to the above restriction.

The eigenvalues of Eqs. (5), (6), as a function of mr_0, are shown in Fig. 1. Now I would like to discuss the results and their physical significance. First let us concentrate on

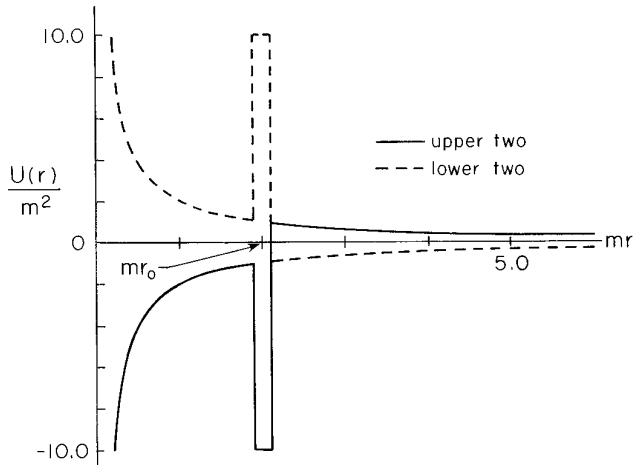

FIG. 2. The graphical representation of the "potentials" for the grand spin zero triplet spin-isospin states $\psi^0_{t,(-)^1}$ in Eq. (6), when $\theta_0 = \pi/2$. The centrifugal term is not included. The "upper two" and "lower two" refer to $\beta = 1$ and $\beta = -1$, respectively. The δ-function is represented by a narrow deep well (high barrier) of area -1 $(+1)$, when it is attractive (repulsive). Note that as $r_0 \to 0$, the potentials for $\beta = \pm 1$ cases approach $\pm 2/r$, respectively.

the $k = 0$ case, whose states have been denoted by $\psi^0_{t,(-)^1}$, which are simpler and are the solutions to Eq. (6). The "potentials" for this equation are depicted in Fig. 2.[1] The potentials in each case consist of attractive and repulsive $2/r$ pieces separated by δ-functions. In the "lower two" case we see that as $r_0 \to 0$, the potential becomes $-2/r$, which is Coulombic and the ground state energy can be directly written down in analogy with the hydrogen atom p-state and gives $E^2 = 0.750m^2$. As r_0 increases from zero, the attractive region of the potential is monotonically reduced and E^2 should approach m^2, as $r_0 \to \infty$. It is worth mentioning that the repulsive δ-function does not change the energy significantly since the wavefunction can partially save itself from it by forming a sharp dimple at that position. One can see that this qualitative argument is completely consistent with the results shown in Fig. 1.

Before I discuss the expected behavior of E^2 for the $k = 0$, "upper two" case, I would like to discuss the effects of the attractive δ-functions. The potentials for $\psi^{k,m}_{t,(-)^k}$, given in Eq. (4), are only δ-functions with coefficients $\pm 2m$. As shown in Ref. [7], for the attractive δ-functions, for small values of r_0 there are no bound states and as r_0 increases one bound state appears and as $r_0 \to \infty$, the value of $E^2 \to 0$ for all values of k (the lower the value of k, the lower the value of E^2). That is, the strength of the "δ-shell" potential increases as the radius of the shell is increased. Now we can analyze the qualitative behavior of E^2 for the $k = 0$, "upper two" case shown in Fig. 1. When $r_0 = 0$, the potential for the "upper two" is $2/r$ and no bound state exists. As r_0 is increased, the potential acquires a negative piece and for r_0 large enough one bound state appears. As $r_0 \to \infty$, the potential becomes $-2/r$ plus the attractive "δ-shell" at infinity. The $-2/r$ piece wants to pull down E^2 to $0.750m^2$; however, with the help of the "δ-shell" piece, E^2 should be pulled down even lower. The results shown in Fig. 1 confirms this qualitative argument and indicates that E^2 is actually pulled down to 0, as $r_0 \to \infty$.

The case of $\psi^{k,m}_{t,(-)^{k+1}}$, which are the solutions to Eq. (5) for $k \geq 1$, is more complicated because there are two coupled second-order equations and the potentials on the diagonals and off-diagonals have different coefficients with opposite signs. Also the δ-functions have different signs even on the diagonals. When $r_0 = 0$, the analytical result recorded in Eq. (7) gives $E^2 = \{0.750, 0.889\}m^2$ for the "lower two" $k = \{1, 2\}$, respectively, and $E^2 = m^2$ for the "upper two." When $r_0 = \infty$, in the absence of the δ-functions, again we can use those analytic results, except that the roles of the "upper" and "lower" are reversed. The results shown in Fig. 1 agree with the analytic result for $r_0 = 0$. We can note that as $r_0 \to \infty$, the δ-functions must be responsible for dragging all of the levels down to zero, even though there are partial cancellations between them.

[1] The "potentials" here are analogous to the ones in the Schrödinger case except that they are in units of (energy)^2. Also the "potentials" discussed here do not include the centrifugal term. Henceforth, I will drop the quotation marks for them.

ACKNOWLEDGMENTS

I thank Professor E. C. G. Sudarshan for very useful discussions. I also acknowledge Professor L. Tuckerman and Professor R. de la Llave for very useful discussions about the numerical methods. This research was supported in part by Department of Energy Grant DE-FG05-85ER40200.

REFERENCES

1. W. H. Press, *Numerical Recipes, The Art of Scientific computing* (Cambridge Univ. Press, Cambridge, UK, 1989).
2. T. H. R. Skyrme, *Proc. R. Soc. London A* **260,** 127 (1961); *Nucl. Phys.* **31,** 556 (1962); *J. Math. Phys.* **12,** 1735 (1971).
3. See, for example, J. G. Williams, *J. Math. Phys.* **11,** 2611 (1970); G. S. Adkins, C. R. Nappi, and E. Witten, *Nucl. Phys. B* **228,** 552 (1983); G. S. Adkins and C. R. Nappi, *Nucl. Phys. B* **233,** 109 (1984); J. Goldstone and R. L. Jaffe, *Phys. Rev. Lett.* **51,** 1518 (1983); I. J. R. Aitchison, C. M. Fraser, and J. A. Zuk, *Phys. Lett. B* **137,** 103 (1984); S. Kahana and G. Ripka, *Nucl. Phys. A* **429,** 462 (1984); E. D'Hoker and E. Farhi, *Phys. Lett. B* **134,** 86 (1984); I. J. R. Aitchison, *Acta Phys. Pol. B* **18,** 207 (1987).
4. E. Witten, *Nucl. Phys. B* **223,** 423, 433 (1983).
5. J. Goldstone and F. Wilczek, *Phys. Rev. Lett.* **47,** 986 (1981).
6. R. MacKenzie and F. Wilczek, *Phys. Rev. D* **30,** 2194 (1984).

7. S. S. Gousheh, *Phys. Rev. D* **45,** 2920 (1992).
8. S. S. Gousheh and R. López-Mobilia, *Nucl. Phys. B* **428,** 189 (1994).
9. A. D. Raptis and J. R. Cash, *Comput. Phys. Commun.* **44,** 95 (1987).
10. A. D. Raptis and J. R. Cash, *Comput. Phys. Commun.* **36,** 113 (1985).
11. J. R. Cash and A. D. Raptis, *Comput. Phys. Commun.* **33,** 299 (1984).
12. T. E. Simos, *J. Comput. Phys.* **108,** 175 (1993).
13. P. J. Prince and J. R. Dormand, *J. Comput. Appl. Math.* **7,** No. 1, 67 (1981).
14. J. R. Dormand, M. E. A. El-Mikkawy, and P. J. Prince, *IMA J. Numer. Anal.* **7,** 423 (1987).