## A B-spline Galerkin method for the Dirac equation

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(Dated: November 5, 2018)

The B-spline Galerkin method is investigated for the simple eigenvalue problem,  $y'' = -\lambda^2 y$ . Special attention is give to boundary conditions. From this analysis, we propose a stable method for the Dirac equation and evaluate its accuracy by comparing the computed and exact R-matrix for a wide range of nuclear charges Z and angular quantum numbers  $\kappa$ . No spurious solutions were found and excellent agreement was obtained for the R-matrix.

The B-spline methods Johnson and Sapirstein [1, 2] introduced into relativistic many-body perturbation theorv have produced results of unprecedented accuracy [3]. Essentially, the local non-orthogonal B-spline basis was transformed to an orthogonal orbital basis by the application of the Galerkin method to the Dirac equation over a finite interval [4]. The resulting basis was finite and effectively complete. Though the low-energy bound states were good approximations to solutions of the Dirac equation, no physical interpretation was important for continuum states. Rapidly oscillating solutions were observed but played a negligible role in the summation over states in their applications [2]. However, these spurious states perturbed the spectrum and slowed the convergence of quantum electrodynamic (QED) calculations. This led Shabaev et al. [5] to propose a dual kinetic balance basis similar to the basis Quiney et al. [6] employed with analytic Slater type functions. Boundary conditions were for the case of a finite nuclear-charge distribution, with the point nucleus considered as a limiting case. Different boundary conditions at the origin were proposed for positive and negative values of  $\kappa$  and both large and small components were set to zero at the large r boundary. Recently Igarashi [7] investigated a variety of methods and boundary conditions. He pointed out that the four boundary conditions used by Froese Fischer and Parpia [8] were excessive and explored the use of B-splines of different order,  $k_p$  and  $k_q$ , as a way of avoiding spurious solutions. In a subsequent paper he concluded that kinetic balance also provided a good basis [9]. No best method was identified. All his methods employed analytic weighting factors to B-spline expansions in order to control the asymptotic properties of large and small components.

R-matrix methods (see Ref.'s [10, 11] for recent reviews) differ from the applications considered by the above authors in that zero boundary conditions at large r, such as proposed by Shabaev *et al.* [5], cannot be used. R-matrix theory assumes an inner region r < a in which exchange is important and an outer region r > a where exchange with an outer electron can be neglected. What is needed is a basis for the inner region that satisfies certain conditions at the r = a boundary. B-splines were very successfully employed in the non-relativistic R-matrix calculations [12], however, they cannot be used in the Dirac-based calculations when spurious states in the continuum spectrum are present. At the same time, the kinetically balanced bases lead to extensive computational difficultes in many-electron calculations.

Spline methods are based on approximation theory. The grid that is selected along with boundary conditions determine a piecewise polynomial space with a finite basis. The unique B-spline basis has many advantages [12, 13], but there are many possible bases. The transformation from a non-orthogonal basis to an orthogonal orbital basis depends on how the Galerkin method is applied. In this letter we propose a simple method for the Dirac matrix equation and apply it to the calculation of the R-matrix boundary condition. All calculations are for a point nucleus so that results can be compared with exact solutions. Special attention is given to the boundary conditions. We also show the relationship between kinetic balance and the use of splines of different order.

At large values of r, the non-relativistic Schrödinger equation has the same form as

$$y''(r) = -\lambda^2 y(r), \ y(0) = 0, \tag{1}$$

for which the solutions are  $y(r) = c \sin(\lambda r)$ . A second boundary condition at r = a defines the allowed values of  $\lambda$ . With y(a) = 0, the values of  $\lambda$  are such that  $\lambda a = n\pi$ and n an integer. We will denote the computed value of n as  $n^*$ .

With a grid consisting of subintervals of length h and knots of multiplicity k at r = 0 and r = a, the solution  $y(r) = \sum_{2}^{N-1} y_i B_i(r)$  satisfies y(0) = y(a) = 0, where N is the size of the basis. The Galerkin requirement that the residual be orthogonal to each basis element in the expansion, leads to the generalized matrix eigenvalue problem

$$D^{(02)} y = -\lambda^2 B y \tag{2}$$

where  $D^{(02)}(i,j) = \langle B_i(r)|B''_j(r)\rangle$  and  $B(i,j) = \langle B_i(r)|B_j(r)\rangle$ . The superscripts on the the derivative matrix designate the order of the derivatives acting on  $B_i(r)$  and  $B_j(r)$ , respectively. The top graph of Fig. 1

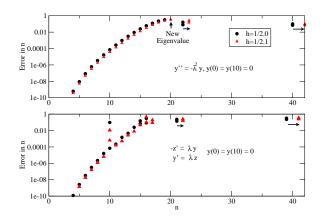


FIG. 1: Errors in n for the Galerkin method applied to equivalent systems of differential equations.

shows the error  $|n - n^*|$  as a function of n for two different grids that increase the matrix size by one. Splines of order 6 were used. The steady reduction in accuracy as n increases is expected but not all solutions are approximations to solutions of the differential equation for which a notion of convergence should apply. As h is reduced and the size of the matrix increased by one, a new eigenvalue appears but the four highest move to higher values. The latter four are not approximations to the differential equation but are needed for the completeness of the orthogonal basis set.

The second-order differential equation can also be written as a pair of first-order equations in a form similar to that of the Dirac equation, namely

$$\begin{bmatrix} 0 & -d/dr \\ d/dr & 0 \end{bmatrix} \begin{bmatrix} y(r) \\ z(r) \end{bmatrix} = k \begin{bmatrix} y(r) \\ z(r) \end{bmatrix}.$$
 (3)

The solution of these equations with y(0) = 0 are  $y(r) = c \sin(kr)$  and  $z(r) = c \cos(kr)$ . Note that the boundary condition y(0) = 0 implies z(0) = c and y(a) = 0 implies  $z(a) = \pm c$ . Thus no boundary condition should be applied on the latter. With the assumption

$$y(r) = \sum_{i=2}^{N-1} y_i B_i(r) \text{ and } z(r) = \sum_{i=1}^N z_i B_i(r),$$
 (4)

the Galerkin method leads to the generalized eigenvalue problem

$$\begin{bmatrix} 0 & D^{(10)} \\ D^{(01)} & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} = k \begin{bmatrix} B & 0 \\ 0 & B \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix}.$$
 (5)

with  $D^{(01)}$  a rectangular matrix of N rows and N-2 columns and  $D^{(10)}$  its transpose. The values of  $\lambda$  occur in positive and negative pairs except for two eigenvalues with  $\lambda = 0$ , a consequence of  $D^{(01)}$  being rectangular. The bottom graph of Fig. 1 shows the errors in *n* for the positive eigenvalues. Note the presence of two solutions for n = 10, 15, 16 and higher. The error of only one

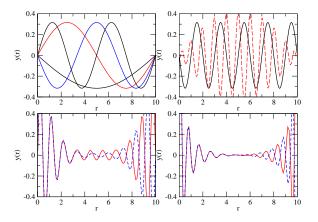


FIG. 2: Some solutions of -z'(r) = ky(r), y'(r) = kz(r) with y(0) = y(10) = 0: top left, n = 1 - 4; top right, n = 10, 10; bottom left, n = 21, 21; bottom right, n = 39, 39 (see Fig. 1).

of the two solutions decreased as the step-size was made smaller. Fig. 2 shows some of the eigenfunctions. Solutions of the differential equation have constant amplitude as seen for n = 1 - 4. Of the two n = 10 solutions, one has constant amplitude whereas the other does not and is referred to as a spurious solution. The four eigenfunctions of the bottom graphs are "border" solutions and correspond to solutions in Fig. 1 that move to higher energies as h is decreased. The numerical properties of the solutions of the two equivalent differential equations can be interpreted by comparing the errors depicted in Fig. 1 as h is decreased and the matrix size increases by one. In the top graph, the errors of all eigensolutions decrease, a new solution appears, and border solutions move to higher energies. In the bottom graph some errors decrease, the new eigensolution may be a spurious solution, and border solutions move to higher energy. Clearly the second-order differential equation solution whose errors are depicted in the top graph is the preferred solution.

Unlike the differential equations where z(r) can be eliminated to yield the original second-order differential equation, the elimination of the vector z leads to the matrix  $D^{(10)}B^{-1}D^{(01)}$  for y that is quite different from  $D^{(02)}$ . Whereas the latter matrix for the B-spline basis is banded, the former is a full matrix. The difference is most dramatic if the matrices are evaluated in the basis of eigenvectors of  $D^{(02)}$ . Then  $D^{(02)}$  is diagonal whereas  $D^{(10)}B^{-1}D^{(01)}$  is striated with a non-zero diagonal and alternating zero and non-zero sub- or super-diagonals.

The pair of first-order equations could also be solved by assuming

$$y(r) = \sum_{i=2}^{N-1} y_i B_i(r)$$
 and  $z(r) = \sum_{i=2}^{N-1} z_i B'(r)$ .

Then the application of the Galerkin method leads to

$$\begin{bmatrix} 0 & D^{(11)} \\ D^{(11)} & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} = k \begin{bmatrix} B & 0 \\ 0 & D^{(11)} \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix}.$$
(6)

Furthermore,  $D^{(11)}$  is symmetric and positive definite. Thus the second set of equations defines the relationship between the expansion coefficients, namely  $y_i = kz_i$  and the equation for y is the same as for  $y'' = -\lambda^2 y$  since, with our boundary conditions,  $D^{(02)} = -D^{(11)}$ . The numerical results are identical.

Each basis function,  $B'_i(r), i = 2, ..., N$  is a spline of order k - 1. This set defines a complete, linearly independent basis for a spline approximation of order k - 1(for simplicity, the superscript k is omitted for splines of order k). Another basis for splines of order k - 1 are the B-splines,  $B_i^{k-1}(r), i = 1, ..., N - 1$ . In fact, the first derivative of a spline function can be found by differencing its B-spline coefficients [14]. Thus this method is similar to the method proposed by Igarashi [7] provided  $|k_p - k_q| = 1$  and without analytic weighting factors. An expansion in the (B, B') basis is also similar to a kinetically balanced basis with  $\kappa = 0$  and is equivalent to an expansion in the  $(B^k, B^{k-1})$  basis. The advantage of the latter is that all basis functions are again strictly positive functions and boundary conditions are simpler to apply.

Some further comments are in order. If in Eq. (2), the matrix  $D^{(02)}$  is replaced by  $-D^{11}$ , no boundary condition is needed to preserve symmetry at r = a. These two matrices differ only in the last column and the difference can be treated as a symmetrizing Bloch operator [12]. The resulting spectrum is for  $n = 1/2, 3/2, \ldots$  for which y'(a) = 0. The numerical accuracy of the modified Eq.(2) and extended Eq. (6) is unchanged.

Based on the above findings for B-spline solutions of differential equations we propose a general, stable method for the Dirac equation and describe its application to the R-matrix method. For a single electron in the Coulomb potential, V(r) = -Z/r, and a point nucleus of charge Z the equation may be written as

$$\begin{bmatrix} V(r) & -c\left[\frac{d}{dr} - \frac{\kappa}{r}\right] \\ c\left[\frac{d}{dr} + \frac{\kappa}{r}\right] & V(r) - 2c^2 \end{bmatrix} \begin{bmatrix} P(r) \\ Q(r) \end{bmatrix} = E\begin{bmatrix} P(r) \\ Q(r) \end{bmatrix}.$$
 (7)

The R-matrix method requires an effectively complete basis  $(P_i, Q_i)$  for the inner r < a region with  $P_i(0) = 0$ and special boundary conditions at r = a that determine the set of energies  $E_i$ . For low positive energies E, and r = a sufficiently large so that V(a) is small relative to  $-2c^2$ , it follows that  $Q(a) \approx (aP'(a) + \kappa P(a))/2ac$  [15]. The boundary conditions for the desired R-matrix solutions of the Dirac equation are  $Q_i(a)/P_i(a) = (b + \kappa)/(2ac) = p$ , where b is an arbitrary constant. Thus both large and small components are non-zero on the boundary though not equal.

With non-zero solutions on the boundary, the Galerkin method as described earlier will not yield a symmetric matrix. Variational methods applied to an associated action ([4], Eq. 7) can be used, but in R-matrix theory it is customary to apply a Bloch operator that enforces the boundary condition as well as symmetry. This operator is then also used for the outer region. Let

$$\hat{\mathcal{H}} = \mathcal{H} + \mathcal{L} \tag{8}$$

where  $\mathcal{H}$  is the Dirac operator of Eq. (7) and  $\mathcal{L}$  is the Bloch operator [16]

$$\mathcal{L} = c\delta(r-a) \begin{pmatrix} -p\eta & \eta\\ (\eta-1) & (1-\eta)/p \end{pmatrix}, \tag{9}$$

and  $\eta$  is an arbitrary constant. In the present calculations we have used the values  $\eta = 0.5$  and  $p = \kappa/2ac$ .

Having defined the operators, let us now define the spline expansions. Suppose there are two sets of B-splines on the same grid that define the  $(B^{k_p}, B^{k_q})$  basis for the Dirac equation. Then the number of functions in each set are  $n_p = n_v + k_p - 1$  and  $n_q = n_v + k_q - 1$ , respectively where  $n_v$  is the number of intervals. The expansions  $P(r) = \sum_{i=2}^{n_p} p_i B_i(k_p; r) \ Q(r) = \sum_{i=1}^{i=n_q} q_i B_i(k_q; r)$  satisfy the boundary condition P(0) = 0 and lead to

$$\begin{bmatrix} V_{11} & W_{12} \\ W_{21} & V_{22} \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} = E \begin{bmatrix} B_{11} & 0 \\ 0 & B_{22} \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix}, \quad (10)$$

where

$$V_{11}(i,j) = \langle B_i^{k_p} | -Z/r | B_j^{k_p} \rangle - (cp/2) \delta_{in_p} \delta_{jn_p}$$
  

$$V_{22}(i,j) = \langle B_i^{k_q} | -Z/r - 2c^2 | B_j^{k_q} \rangle + (c/2p) \delta_{in_q} \delta_{jn_q}$$
  

$$W_{12}(i,j) = -c \langle B_i^{k_p} | \frac{d}{dr} - \frac{\kappa}{r} | B_j^{k_q} \rangle + (c/2) \delta_{in_p} \delta_{jn_q}$$
  

$$W_{21}(j,i) = c \langle B_j^{k_q} | \frac{d}{dr} + \frac{\kappa}{r} | B_i^{k_p} \rangle - (c/2) \delta_{in_q} \delta_{jn_p}, \quad (11)$$

and  $B_{11}$  and  $B_{22}$  are the overlap matrices for  $B^{k_p}$  and  $B^{k_q}$ , respectively. We have used the fact that for a grid with muliple knots at r = a,  $B_N(a) = 1$  for all orders.

From the above finite set of solutions, an R-matrix relation can be derived that connects the inner and outer region. For a given energy E, the relation has the form

$$P(a) = \left[ R(E) - \frac{b + \kappa}{(b + \kappa)^2 + (2ac)^2} \right] \left[ 2acQ(a) - (b + \kappa)P(a) \right]$$
(12)

where the relativistic R-matrix is defined as

$$R(E) = \frac{1}{2a} \sum_{i} \frac{P_i(a)P_i(a)}{E_i - E}.$$
 (13)

Eq. (12) contains the correction  $(b+\kappa)[(b+\kappa)^2+(2ac)^2]$ , first obtained by Szmytkowski and Hinze [16]. This correction is due to the fact that the set of relativistic basis functions  $(P_i, Q_i)$  is incomplete on the surface r = a. However, it is small in most realistic cases and usually is omitted.

If we employ expansions with  $k_q = k_p$  in Eq. (10), many pseudo-solutions are found in the positive-energy spectrum. These pseudo-solutions are characterized by

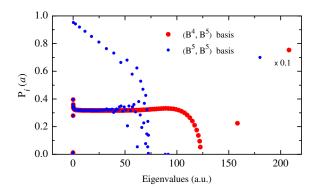


FIG. 3: Comparison of the surface amplitudes for  $(B^4, B^5)$ and  $(B^5, B^5)$  bases in the case Z=1,  $\kappa = -1$ , a = 20, N = 100, on an equally spaced grid.

a rapidly oscillating behavior with every coefficient in the B-spline expansion changing sign: they cannot be used directly in Eq. (13) for the R-matrix. The use of B-splines of different order removes all pseudo-solutions. The  $(B^k, B^{k+1})$  basis was found to be the most stable numerically. This stability is extremely important for the calculation of R(E). Fig. 3 compares the surface amplitudes  $P_i(a)$ . In the case of the  $(B^4, B^5)$  basis the surface amplitudes vary smoothly with energy, whereas the  $(B^5, B^5)$  basis produces many pseudo-solutions with large surface amplitudes. The surface amplitudes for these two calculations agree only for some low energy eigenstates, but differ considerably in the higher energy spectrum. The high energy eigensolutions in both cases are not pseudo-solutions, though they have very large surface amplitudes. As in the model equation, these border solutions are needed for the effective completeness in the transformation from a B-spline basis to eigenstates of the Dirac matrix equation. These eigenstates provide a relatively large contribution to the total value of R(E)that brings the final value in closer agreement with the exact value. Note that Fig. 3 shows only positive-energy (electron) solutions. Contributions to the R-matrix (13) from the negative-energy (positron) solutions were found to be negligibly small in the present case.

In the case of the Dirac-Coulomb problem with a point nucleus, we can check directly the accuracy of the resulting R-matrix because the wavefunctions are known analytically. The R-matrix can be expressed as

$$R(E) = \left[2acG\left(E\right) - \left(b + \kappa\right)F\left(E\right)\right]/F(E), \qquad (14)$$

where F(E) and G(E) are the large and small components of the Dirac-Coulomb wavefunction for given  $\kappa$  and Z. Comparison of the exact R-matrix with the one obtained from B-spline bases is shown in Fig. 4. There is very close agreement with the exact results for a wide range of energy for the  $(B^4, B^5)$  basis (only the lowenergy region is shown for better visualization). The

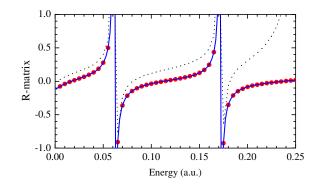


FIG. 4: Comparison of the exact R-matrix (blue line) with B-spline R-matrix in the  $(B^4, B^5)$  basis (red circles) and in the  $(B^5, B^5)$  basis (dotted line) for the same case as Fig. 3.

results correctly reproduce the tangent-like behavior of the exact R-matrix, along with a correct representation of all poles. At the same time, the  $(B^5, B^5)$  basis lead to large errors due to the presence of pseudo-states.

The  $(B^4, B^5)$  method with a = 20/Z and N = 100was checked for a wide range of Z and with  $\kappa$  up to  $\pm 50$ . No spurious solutions were found. The accuracy of the R-matrix for small Z and all  $\kappa$  was in the range  $10^{-6}$  to  $10^{-8}$ , decreasing for large Z. At Z = 100 the accuracy had deteriorated to  $10^{-3}$  but no attempt was made to modify the grid or change  $(k_p, k_q)$ . The R-matrix was relatively independent of whether an equally spaced or exponential grid was used although the behavior near the origin was not monitored.

We have also checked the accuracy of the R-matrix calculations for the kinetic balance B-spline basis proposed by Igarashi [9] but omitting analytic factors. The resulting accuracy is approximately the same as for  $(B^k, B^{k+1})$ or (B, B') bases but the method is much more difficult to implement, especially in the case of multi-channel Rmatrix calculations, since different bases are needed for different values of  $\kappa$ . The dual kinetic balance basis, proposed by Shabaev et al. [5] failed to reproduce an accurate R-matrix, because it resulted in many pseudosolutions in the non-physical energy region just above the  $-mc^2$  threshold. We also found that the appearance of pseudo-solutions depends only in a minor way on initial or boundary conditions. In fact the most accurate results are obtained with a minimum of additional conditions on the B-spline coefficients.

In conclusion, a simple but stable method is proposed for the solution of the Dirac equation, including the eigenvalue problems arising in R-matrix theory. Whereas earlier considerations concentrated on the non-relativistic limit of the Dirac equation, we have shown the importance of the large r region. Any reliable method for the Dirac equation must be able to solve the pair of first-order equations of Eq.(3) to the same accuracy as Eq.(2) or, equivalently have matrices for which  $D^{(02)} =$   $D^{(10)}B^{-1}D^{(01)}$ . In general, accurate methods require an exponential grid near the origin in order to reproduce the  $r^{\gamma}$  behavior where  $\gamma = \sqrt{\kappa^2 - Z^2/c^2}$  but the singularity at the origin itself has not been found to be a problem.

The methods described here have been applied to the investigation of low-energy electron scattering from Cs [11]. A finite nucleus was used along with B-splines of order (8,9). Close agreement with experiment was obtained for the total and angle differential cross sections as well as several spin-asymmetry parameters.

The work of O. Z. was supported by the National Science Foundation under Grant No. PHY-0244470.

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