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Perturbative Solutions of Quantum Mechanical Problems by Symbolic Computation

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Symbolic computation provides excellent tools for solving quantum mechanical problems by perturbation theory. The techniques presented herein avoid the use of an infinite basis set and some of the complications of degenerate perturbation theory. The algorithms are expressed in the Maple symbolic computation system and solve for both the eigenfunctions and eigenenergies as power series in the order parameter. Further, each coefficient of the perturbation series is obtained in closed form. In particular, this paper examines the application of these techniques to R. A. Moore's method for solving the radial Dirac equation. One is confident that the techniques presented will also be useful in other applications.

1. INTRODUCTION

The purpose of this work is multifold. One aspect is to demonstrate the applicability and usefulness of symbolic computation for the analysis of certain physical problems. Another is to present the solution to a realistic non-trivial problem. Finally, a number of derivations and procedures required for the above analysis are given.

There are a number of reasons for considering the present approach. Most physical problems of current interest cannot be solved exactly in analytic form but

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require some approximation techniques, such as Rayleigh–Schrödinger perturbation theory for quantum problems. A known difficulty with the conventional approach to perturbation theory, which uses a set of basis functions, is that computations beyond first order in the eigenenergies become impossibly tedious. In the event that higher order terms are important, it is of interest to develop suitable methods to obtain their solutions. Further, once one has a method substantiated for a certain class of problems, its extension to more complicated problems can be made with some confidence. In addition, analytic results can be used to test numerical procedures required in situations where analytic results do not exist.

Since a rather diverse set of concepts and procedures are combined, that is, symbolic computation, quantum mechanical perturbation theory, methods for solving ordinary differential equations (e.g., the methods of "variation of parameters" and ladder operators) and computationally efficient formulas, a rather detailed survey is presented.

The Maple [1] symbolic computation system is used because it is available to the authors and because it is suitable for the type of problems considered. Other symbolic computation systems may also be applicable. It will be shown that it is not always necessary to resort to numerical procedures in order to solve higher order perturbative equations. The advantage of symbolic computation is that one can obtain a series solution in which *each term of the series is in closed form*. Another advantage occurs when the series in question is slowly convergent or divergent. In such cases Padé techniques are usually applied. However, numerical instabilities are often encountered when the Padé values are calculated by floating-point arithmetic. This occurs when the results are sensitive to round off errors [2, p. 613]. In this event, the results become unreliable and inconclusive. An algebraic solution avoids such difficulties.

The particular physical problem analysed is the one-particle Dirac equation for hydrogen-like atoms. There are a number of reasons for this choice. First, exact solutions exist, e.g., [3], and hence, any approximate solution can be validated at each step. Second, this problem is sufficiently complex so that the methods applicable to it should suffice for similar yet more complicated problems. Third, a perturbative formulation exists which has received some analytic treatment [4–9] and numerical evaluation [10] to low order. The problem and the perturbative scheme are reviewed in Section 2. The zeroth and first-order solutions are summarized in Section 3 so that the notation can be specified, the operators defined, and a number of relevant expressions be readily available. Finally, in this section the inhomogeneous equations that must be solved at the jth order and the corresponding energy contributions are defined.

Because the total angular momentum commutes with the Hamiltonian, the eigenfunctions can be written in terms of products of radial functions and angular momentum functions. In this case, the inhomogeneous equations reduce to ordinary differential equations in the radial variable. The methods employed in this work are reviewed in Section 4.

It is well known that, when the eigenfunction is known to a given order, $O(j)$, say, the eigenenergy can be determined to order $O(2j+1)$. This result and the eigenfunction normalization are used to generate computationally efficient energy formulas. These are given and discussed in Section 5.

Having specified the quantities to be calculated, the next step was to perform the actual computations. The important details of the Maple programs used are presented and discussed in Section 6. These programs generate a number of results which are given, analysed, and discussed in Section 7. The eigenfunctions have been computed for the first 16 states up to and including the fifth order and, hence, their eigenenergies computed to eleventh order. The eigenenergy results are compared to other works and in all instances exact agreement is found with the power series expansion in terms of the fine structure constant, α, of the exact eigenenergy. Thus the concerns raised by Tomishima [7] are completely negated and the validity of the procedure established. It is anticipated that this procedure will be useful for other problems. In addition, a procedure is outlined by which possible exact solutions to the eigenenergies may be inferred from a few of the leading terms of a perturbative calculation. Next, the matrix elements appropriate for the Stark effect and the electric dipole transitions are evaluated and the coefficients of the α^0 and α^2 terms tabulated. The analytic results again verify the previous numerical results [10]. Finally, the hyperfine splitting is evaluated with these analytic results verifying the previous numerical results [10]. In this way, the concept of being able to calculate the coefficients in α^2 expansions with some accuracy is justified for particular well defined problems.

The application to other systems is discussed briefly in Section 8 and the paper closes, Section 9, with a few comments and conclusions.

2. MOORE'S DECOUPLING TECHNIQUE FOR THE ONE-PARTICLE DIRAC EQUATION

2.1. *The Hierarchy of Equations*

Starting with the one-particle Dirac equation

$$(c\vec{\alpha}\cdot\vec{\mathbf{p}}+\beta m_0c^2+IV)\Phi=E\Phi, \tag{1}$$

where the notation is defined in [4], the Hamiltonian is rewritten as

$$\hat{H}=\hat{H}_0+\lambda\hat{H}_1, \tag{2}$$

where

$$\hat{H}_0=c\vec{\alpha}\cdot\vec{\mathbf{p}}+\beta m_0c^2+\tfrac{1}{2}(I+\beta)V$$

and

$$\hat{H}_1=\frac{1}{\alpha^2}\hat{H}'_1=\frac{1}{2\alpha^2}(I-\beta)V.$$

Now the problem is treated formally as though $\hat{H}_1$ were a perturbation with λ being the usual order parameter but to be evaluated at $\lambda = \alpha^2$. Thus, both the energy and eigenfunctions are written as

$$E = (E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots) = \sum_{p=0}^{\infty} \lambda^p E_p \tag{3}$$

$$\Phi = (\Phi^0 + \lambda \Phi^1 + \lambda^2 \Phi^2 + \cdots) = \sum_{p=0}^{\infty} \lambda^p \Phi^p. \tag{4}$$

Moore's hierarchy of equations is obtained by applying formal Rayleigh–Schrödinger perturbation theory to the eigenvalue equation giving

$$\begin{aligned}
&\lambda^0\colon\ \hat{H}_0 \Phi^0 = E_0 \Phi^0 \\
&\lambda^1\colon\ \hat{H}_0 \Phi^1 + \hat{H}_1 \Phi^0 = E_0 \Phi^1 + E_1 \Phi^0 \\
&\lambda^2\colon\ \hat{H}_0 \Phi^2 + \hat{H}_1 \Phi^1 = E_0 \Phi^2 + E_1 \Phi^1 + E_2 \Phi^0 \\
&\ \vdots \\
&\lambda^j\colon\ \hat{H}_0 \Phi^j + \hat{H}_1 \Phi^{j-1} = \sum_{i=0}^{j} E_i \Phi^{j-i}
\end{aligned} \tag{5}$$

etc. Note that $\hat{H}'_1$ is the perturbation in Moore's work [4–6] and that the fine-structure constant in the scheme presented here is used both as a constant and to fix the final value assumed by λ. Therefore, the various terms in the perturbative expansions such as the energies E_0, E_1, etc. will also depend on α. To understand the hierarchy, one must carefully recognise this distinction between the two roles played by the fine structure constant. For spherically symmetric potentials, $V(r)$, the familiar angular momentum operator $\hat{K}$ commutes with both $\hat{H}_0$ and $\hat{H}_1$. Therefore, one can separate the wave function into its respective radial and spin-angular components as usual.

3. LOW-ORDER SOLUTIONS FOR HYDROGEN-LIKE ATOMS

3.1. *Zero-Order Solution*

The low-order solutions to a hydrogen-like atom are reviewed in this section in order to have certain expressions at hand and to set the notation. More details can be found in [4–6, 8–10]. Letting

$$\Phi^0 = A \begin{pmatrix} \Psi_1^0 \\ \Psi_2^0 \end{pmatrix} \tag{6}$$

in the λ^0 equation of (5), where Ψ_1^0 and Ψ_2^0 are two-component spinors and A is some constant allowing Φ^0 to be normalised when Ψ_1^0 is normalised,

$$\Psi_2^0 = c \frac{\vec{\sigma} \cdot \vec{\mathbf{p}}}{(E_0 + m_0 c^2)} \Psi_1^0 \tag{7}$$

and

$$c\vec{\sigma}\cdot\hat{\mathbf{p}}\Psi_2^0 + V\Psi_1^0 = \varepsilon_0\Psi_1^0, \tag{8}$$

where $\varepsilon_0 = E_0 - m_0c^2$ and $V(r) = -Ze^2/r$, the hydrogen-like potential. Eliminating Ψ_2^0 gives

$$\left\{\frac{p^2}{2m_0} + \left(1 + \frac{\varepsilon_0}{2m_0c^2}\right)(V - \varepsilon_0)\right\}\Psi_1^0 = L(p)\,\Psi_1^0 = 0. \tag{9}$$

The exact solution becomes obvious by setting

$$\Psi_1^0 = R_1^0(r)\,\psi_{lm\kappa}^1 \tag{10}$$

which makes, see (7),

$$\Psi_2^0 = R_2^0(r)\,\psi_{lm\kappa}^2, \tag{11}$$

where the $\psi_{lm\kappa}^i$ are the spin-angular functions of $\hat{K}$ [4, p. 1243]. Defining

$$Z' = \left(1 + \frac{\varepsilon_0}{2m_0c^2}\right)Z \qquad \text{and} \qquad t = 2Z'r/na_0, \tag{12}$$

the radial equation can be written as

$$\left[\frac{d^2}{dt^2} + \frac{2}{t}\frac{d}{dt} - \frac{\kappa(\kappa-1)}{t^2} + \frac{n}{t} - \frac{1}{4}\right]R_1^0 = L(t)\,R_1^0 = 0. \tag{13}$$

Here $\kappa = l + 1$ or $-l$. This is an amazingly simple result for it represents just a hydrogen-like system containing only a slightly renormalized potential and eigenenergy. One has only a one component equation which can be solved exactly! The effective eigenvalue is

$$\varepsilon_0\left(1 + \frac{\varepsilon_0}{2m_0c^2}\right) = -\left(1 + \frac{\varepsilon_0}{2m_0c^2}\right)^2 Z^2\frac{R_H}{n^2}, \qquad n = 1, 2, \ldots. \tag{14}$$

Solving for ε_0 yields

$$\varepsilon_0 = -Z^2\frac{R_H}{n^2}\left(1 + \frac{Z^2\alpha^2}{4n^2}\right)^{-1}, \tag{15}$$

where $R_H = \alpha^2m_0c^2/2$ is the Rydberg energy unit. The normalized radial solutions are

$$R_1^0 = R_{n,l}(t) = \left\{\left(\frac{2Z'}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2} \times t^l e^{-t/2} L_{nl}(t), \tag{16}$$

where the L_{nl}'s are the Laguerre polynomials. R_2^0 is given by

$$R_2^0 = -\frac{i\hbar c}{2m_0 c^2 A^2}\left[\frac{d}{dr} - \frac{(\kappa - 1)}{r}\right] R_1^0. \tag{17}$$

Normalizing Φ^0 requires

$$A^2 = 1 + \frac{\varepsilon_0}{2m_0 c^2}. \tag{18}$$

3.2. *First-Order Solution*

Since both the complete solutions and Φ^0 are eigenfunctions of the total angular momentum operator, the energy E_1 is obtained using non-degenerate perturbation theory:

$$E_1 = \frac{1}{\alpha^2} \langle \Psi_1^0 | \hat{H}_1 | \Psi_1^0 \rangle \tag{19}$$

This can be evaluated exactly [8] to give

$$E_1 = R_H \frac{Z^4}{n^4}\left(1 + \frac{\varepsilon_0}{2m_0 c^2}\right)^2 \left(\frac{1}{2} - \frac{n}{|\kappa|}\right). \tag{20}$$

Collecting E_1 and E_0 and computing the Taylor series expansion in α^2 of (3) gives the eigenenergy E correct to order α^2. The terms of order α^4 can certainly be collected at this point but they will clearly not give the total contribution. To improve the energy calculation, it is necessary to solve the first order equation for Φ^1. Proceeding as with the zero-order equation and setting

$$\Phi_1 = A \begin{pmatrix} \Psi_1^1 \\ \Psi_2^1 \end{pmatrix} \tag{21}$$

then

$$\Psi_2^1 = \frac{1}{m_0 c^2 + E_0}\left(c\vec{\sigma} \cdot \vec{\mathbf{p}} \Psi_1^1 + \frac{V}{\alpha^2} \Psi_2^0 - E_1 \Psi_2^0\right) \tag{22}$$

or, with (7),

$$\Psi_2^1 = \frac{c\vec{\sigma} \cdot \vec{\mathbf{p}}}{(m_0 c^2 + E_0)} \Psi_1^1 + \frac{V c\vec{\sigma} \cdot \vec{\mathbf{p}}}{\alpha^2 (m_0 c^2 + E_0)^2} \Psi_1^0 - \frac{E_1 c\vec{\sigma} \cdot \vec{\mathbf{p}}}{(m_0 c^2 + E_0)^2} \Psi_1^0. \tag{23}$$

The angular dependence of each component is the same, allowing one to write $\Psi_1^1 = R_1^1 \psi_{nl\kappa}^1$ and to proceed as in the previous section. Thus

$$L(t)\, R_1^1 = f(t), \tag{24}$$

where $L(t)$ is given by (13) and

$$f(t) = -\frac{Z^2}{4n^2}\left[\left(\frac{1}{2}-\frac{n}{|\kappa|}\right)A^2 - \frac{4n(\kappa-1)}{t^3} + \frac{4n^2}{t^2} - \frac{n}{t} + \frac{4n}{t^2}\frac{d}{dt}\right]R_1^0$$
$$-\alpha^2\frac{Z^4}{4n^4}A^2\left(\frac{1}{2}-\frac{n}{|\kappa|}\right)\left(\frac{n}{t}-\frac{1}{4}\right)R_1^0. \tag{25}$$

One notes that in Eq. (2.19) of [8], some terms of order α^2 were omitted in $f(t)$.

The exact solution to this equation is given in S. Lee's Master's thesis [9, p. 15] and reported elsewhere [8]. Note that in [8], a term proportional to dR_1^0/dt was omitted since it contributed nothing to calculations of order α^4.

3.3. *Jth-Order Solution*

Proceeding as with the first-order case, set

$$\Phi^j = A\begin{pmatrix}\Psi_1^j \\ \Psi_2^j\end{pmatrix} \quad \text{where} \quad \Psi_k^j = R_k^j \psi_{nl\kappa}^k, \quad k = 1, 2 \tag{26}$$

and obtain for the lower component:

$$\Psi_2^j = \frac{1}{(m_0c^2+E_0)}\left(c\vec{\sigma}\cdot\vec{\mathbf{p}}\,\Psi_1^j + \frac{V}{\alpha^2}\Psi_2^{j-1} - \sum_{i=1}^{j} E_i \Psi_2^{j-i}\right). \tag{27}$$

Now, the equation for the upper component is

$$L(p)\Psi_1^j = \frac{c\vec{\sigma}\cdot\vec{\mathbf{p}}}{2m_0c^2}\left\{\sum_{i=1}^{j} E_i \Psi_2^{j-i} - \frac{V}{\alpha^2}\Psi_2^{j-1}\right\} + A^2\sum_{i=1}^{j} E_i \Psi_1^{j-i}, \tag{28}$$

where $L(p)$ is given in (9). This reducmes to an inhomogeneous equation of the form (24)

$$L(t)R_1^j = f_j(t) \tag{29}$$

with

$$4\varepsilon_0 f_j(t) = -\frac{Z\alpha}{n}\left(\frac{d}{dt}+\frac{\kappa+1}{t}\right)\operatorname{Im}\left(\sum_{i=1}^{j} E_i R_2^{j-i} - \frac{V(t)}{\alpha^2}R_2^{j-1}\right)$$
$$+\sum_{i=1}^{j} E_i R_1^{j-i}.$$

Recalling that the radial function of the lower component is imaginary, just as in the zero-order case in (17), the symbol Im indicates imaginary part of the argument. The potential $V(r)$ is rewritten as $V(t)$.

All the solutions of the inhomogeneous equations are subject to the condition that the final wavefunction Φ be normalised. I.e.,

$$\langle \Phi | \Phi \rangle = 1 \tag{30}$$

by substituting the series solution of (4) into the above, this condition becomes

$$\begin{aligned} \lambda^0&: \quad \langle \Phi^0 | \Phi^0 \rangle = 1 \\ \lambda^1&: \quad \langle \Phi^0 | \Phi^1 \rangle + \langle \Phi^1 | \Phi^0 \rangle = 0 \end{aligned} \tag{31}$$

etc., or generally,

$$\sum_{i=0}^{j} M_i^{j-i} = 0, \qquad \text{where} \quad j = 0\ 1, 2, ...,$$

and

$$M_r^s = \langle \Phi^r | \Phi^s \rangle. \tag{32}$$

Finally, once the various inhomogeneous equations are solved, the jth-order energy can be calculated from the conventional formula:

$$E_j = \langle \Phi^0 | \, \hat{H}_1 \, | \Phi^{j-1} \rangle - \sum_{i=1}^{j-1} E_i M_0^{j-i}. \tag{33}$$

In the next section, a method is presented to systematically solve for any of the various inhomogeneous solutions, without the use of formal degenerate perturbation theory. For the example shown, these are obtained in closed form. The approach uses simple methods of ordinary second-order differential equations.

4. Procedure for Solving the Inhomogeneous Equations

4.1. *Method*

First, consider only the ground state $1s_{1/2}$ ($n = 1$, $l = 0$, and $\kappa = 1$). In this case, the radial eigenfunction (to within a normalisation constant) is simply

$$R_1^0(t) = y_1(t) = e^{-t/2}, \tag{34}$$

which is one solution to the homogeneous equation (13). Note that the latter is *second-order* and can be written in the standard form,

$$\left[\frac{d^2}{dt^2} + P(t) \frac{d}{dt} + Q(t) \right] y(t) = 0, \tag{35}$$

where

$$P(t)=\frac{2}{t} \qquad \text{and} \qquad Q(t)=-\frac{1}{4}+\frac{n}{t}-\frac{\kappa(\kappa-1)}{t^2}.$$

There is another solution, $y_2(t)$, which is linearly independent to $y_1(t)$. Given $y_1(t)$, $y_2(t)$ can be generated by the method of "*reduction of order*" [11, p. 100],

$$y_2(t)=y_1(t)\int\frac{W(t)}{y_1^2}\,dt, \tag{36}$$

where W is the Wronskian,

$$W(t)=W(y_1,y_2)=\exp\left(-\int P(t)\,dt\right)=t^{-2}. \tag{37}$$

For the ground state,

$$y_2(t)=e^{-t/2}Ei(t)-\frac{e^{t/2}}{t}, \tag{38}$$

where $Ei(t)$ is the exponential integral [12, p. 228 (Eq. 5.1.2)]. Although this solution is mathematically present, it is non-square-integrable and, therefore, unphysical. The solution y_2 represents the *ghost state* of the ground state. Each physical eigenfunction has its own "ghost" state and, in all cases, the latter is irregular and thus non-square-integrable. These "ghost" states are well known because they must be included when one solves the Schrödinger equation for the truncated Coulomb potential, a model used by nuclear physicists [13, p. 330]. Now that two independent solutions of the homogenous equation are known, the particular solution to the inhomogeneous equation is given by the method of "*Variation of parameters*" [11, p. 121] and is

$$y_p=u(t)\,y_1(t)+v(t)\,y_2(t), \tag{39}$$

where

$$u(t)=-\int\frac{y_2(t)f(t)}{W(y_1,y_2)}\,dt \qquad \text{and} \qquad v(t)=\int\frac{y_1(t)f(t)}{W(y_1,y_2)}\,dt. \tag{40}$$

If the calculated particular solution y_p is square-integrable, it represents the desired physical solution. In this case, the general solution to the inhomogeneous equation

$$y_G=y_p+C_1y_1+C_2y_2 \tag{41}$$

is given with $C_2=0$ and C_1 being determined by the orthogonality requirement. If the calculated solution y_p is not square-integrable, it is be necessary to add the right amount of "ghost" state y_2, in order to make it square-integrable, that is, $C_2\neq 0$.

Fortunately, this eventuality has not arisen so far in our calculations and, as discussed further on, the particular solution of the jth inhomogeneous equation for the Dirac hydrogen problem is always a square-integrable function, albeit a border-line case.

An important distinction is in order here. In systems such as the nuclear model, the "ghost' states are usually called "companion states" because they appear in the physical solution, the truncation of the Coulomb potential at the origin having ensured that these solutions are square-integrable. No such truncation appears in this application. Although these "ghost" states are used in the calculations they *never appear in the final solution.* It is for this reason that they are called "ghost" states, herein. Note that one could have solved the inhomogeneous equations using Green's functions. An approach similar to the one presented here also uses regular and irregular wavefunctions to construct a Green function solution of the inhomogeneous equation and can be found in the work of Byron and Fuller [14, p. 420). However, this method is more complicated and unnecessary in this particular application.

4.2. *Generation of "Ghost" States Using Ladder Methods*

For the ground state, or any other state where $l = n - 1$, the Legendre polynomial is just a constant and the "ghost" states are easy to calculate using the integration formula of (36). However, this integration rapidly becomes tedious for increasing values of n and low values of l. For instance, for the $3s_{1/2}$ state ($n = 3$, $l = 0$, $\kappa = 1$), one must calculate

$$\int \frac{e^t}{t^2(6 - 6t + t^2)^2}\, dt. \tag{42}$$

To evaluate this integral, the roots of the Legendre polynomial in the denominator of the integrand must be determined. They are $3 \pm \sqrt{3}$. Factoring the denominator and expanding it into partial fractions, the Maple system can be used to integrate the resulting expression, term by term, to yield the ghost state, namely,

$$\frac{1}{36t}\,[(5t - t^3 - 2)e^{t/2} + (6t - 6t^2 + t^3)E_i(t)e^{-t/2}]. \tag{43}$$

This direct interactive method becomes impossible for the $n \geqslant 4$, $l = 0$, $\kappa = 1$ states. A much more efficient algorithm can be obtained by using ladder operators. Infeld and Hull [15] have compiled raising and lowering operators for a large class of physical problems. Their precise definitions for the Whittaker function [12, p. 505] permits one to express the solution of the radial equation for the hydrogen-like atom as

$$R_1^0 = R_{n,l}(t) = \frac{C}{t} \times W_{n,l+1/2}(t), \tag{44}$$

where C is a constant. The raising operator, as given by Eq. (5.1.6b) of their work [15, p. 37], gives

$$R_{n+1,l}(t) = C \times \left(\frac{1}{2} - \frac{n}{t} - \frac{d}{dt}\right) t R_{n,l}(t), \tag{45}$$

where C is determined by normalisation requirements. This ladder operation increments n and leaves l constant. It is found that this same ladder operation works for the set of "ghost" states as well. This is not surprising since nothing in the ladder operator makes explicit use of the requirement that the wave function be normalizable. One proceeds by using the integral in (36) to calculate the "ghost" state for $l = n - 1$. This operation is fairly fast using Maple. For any other "ghost" state of given l, one simply ladders up in n. In our case, the constant is determined so that the Wronskian remains unchanged from its value in (37). This is a highly efficient method for determining the "ghost" states.

5. FORMULAS FOR EFFICIENT ENERGY CALCULATIONS

According to the conventional formula, the third-order energy E_3 is given by

$$E_3 = \frac{1}{\alpha^2} \langle \Phi^0 | \hat{H}_1 | \Phi^2 \rangle - E_1 \langle \Phi^0 | \Phi^2 \rangle \tag{46}$$

which requires the knowledge of Φ to second-order. However, Hylleraas [16] first showed that the third-order energy could be calculated by the wave function to first order and that E_3 is also given by

$$E_3 = \frac{1}{\alpha^2} \langle \Phi^1 | \hat{H}_1 | \Phi^1 \rangle - E_1 \langle \Phi^1 | \Phi^1 \rangle. \tag{47}$$

Furthermore, the knowledge of Φ to second-order is enough to calculate the energies to fourth and fifth order. These are special cases of a well-known result in quantum chemistry, namely, knowing the wave function to order $O(j)$, allows the energies to be calculated to order $O(2j+1)$. Dalgarno and Stewart [17] made explicit demonstrations of this theorem. Hirschfelder *et al.* [18] provide general formulas for the energies calculated for the same normalisation conditions as in (31). The gain in computational efficiency is obvious. The efficient formulas for energies according to our normalisation scheme are given by the following. These are divided into even and odd cases.

$$E_j = \langle \Phi^{p-1} | \hat{H}_1 | \Phi^p \rangle - \sum_{i=1}^{p-1} E_i \sum_{m=1}^{i} M_{p-m}^{p+m-i} + E_p M_0^p,$$

$$\text{where} \quad j = 2p, \quad p = 1, 2, 3, \ldots, \tag{48}$$

with the understanding that the summation is void for $p=1$ and that all the matrix elements are real-valued, and

$$E_j = \langle \Phi^p | \hat{H}_1 | \Phi^p \rangle - \sum_{i=1}^{p} E_i \sum_{m=1}^{i} M_{p-m+1}^{p+m-i},$$

$$\text{where} \quad j = 2p+1, \quad p = 1, 2, 3, \ldots. \tag{49}$$

Exploiting, the orthogonality conditions, (49) can be reduced into a computationally more efficient form,

$$E_j = \langle \Phi^p | \hat{H}_1 | \Phi^p \rangle - \sum_{i=1}^{p} E_i \, g(i, j), \qquad \text{where} \quad j = 2p+1, \quad p = 1, 2, \ldots \tag{50}$$

with

$$g(i, j) = 2 \sum_{m=1}^{i'} M_{p-m+1}^{p+m-i} + M_{p-i'}^{p-i'} \qquad \text{if} \quad i = 2i'+1, \qquad \text{where} \quad i' = 0, 1, 2, 3, \ldots$$

$$g(i, j) = 2 \sum_{m=1}^{i'} M_{p-m+1}^{p+m-i} \qquad \text{if} \quad i = 2i', \qquad \text{where} \quad i' = 1, 2, 3, \ldots.$$

Note that although the odd energy formula in (49) is identical with that of Hirschfelder, there is a slight difference in the formula for the even case. Mathematically, they are equivalent but Hirschfelder's formula requires the computation of $\frac{1}{2}(p^2+p)$ inner products, whereas, ours requires $p-1$ less terms. Apparently, his form does not fully exploit the full reduction that can be obtained by using the orthogonalisation scheme of (32). This may seem a trivial gain since the formulas grow as p^2 for p large. However, as discussed later on, this gain is far from trivial, since the computations of the inner products represent that part of the computer algebra program which requires the most time and memory. The derivation of these efficient energy formulas is given in the Appendix.

There is another type of normalisation which is commonly used. Instead of requiring that $\langle \Psi | \Psi \rangle = 1$, the perturbed components of the wave function are set to be orthogonal, i.e.:

$$\langle \Phi^0 | \Phi^j \rangle = 0 \qquad \text{for} \quad j = 1, 2, \ldots \tag{51}$$

In this case, the energy relations are given by Dupont-Bourdelet *et al.* [19]. However, such a scheme is inefficient if one intends to use the wavefunction in the calculation of matrix elements other than those required for the energies.

Now the solution of the various inhomogeneous equations and the energy coefficients is reduced to calculating a series of definite and indefinite integrals.

6. MAPLE PROGRAMS

In this section a discription is given of the Maple program DIRAC1 which computes the radial wavefunction to order $O(j)$ according to (29) and the eigenenergies to order $O(2j+1)$ according to (48) and (50) for the sample problem examined herein. The listings of these programs are available upon request. The output from these programs and their by-products are discussed in the results section. The reader is referred to the Maple manual [1] for further information about the Maple system. Discussed in this section are the important features of the program, in particular: the Maple algorithms which solve the definite and indefinite integrals and the method employed in the manipulation and reduction of the resulting expressions.

6.1. *Definite Integration*

As mentioned before, the zero-order solution in (16) involves the Laguerre polynomials. The definite integrals required have the form:

$$\int_0^\infty e^{-ut} f(t) L_{nl}(t)\, dt, \tag{52}$$

where the $f(t)$ may also contain a Laguerre polynomial. Although, this term has the desirable feature of generality and was successfully used in low order, it must be pointed out that not all integrals of the form (52) are known or even readily available in tables. Furthermore, one cannot a *priori* expect closed form solutions for the higher order terms for all bound states. If one partially relinquishes this generality and tackles the problem for *only one given state*, the Laguerre polynomial can be broken up and all the various inner products and matrix elements can then be decomposed into a sum of definite integrals of the form

$$\int_0^\infty e^{-ut} t^i \ln^m t\, dt \tag{53}$$

for $u > 0$, $i = 0, 1, \ldots$ and $m = 0, 1, 2, \ldots$. Although one has to compute many more definite integrals, individually, they are much easier to solve. This greatly increases the chance of obtaining a solution. Once the problem has been successfully solved for the ground state, one can then attempt to solve the more difficult problem of a higher state. This would be tedious to do by hand but presents no problem for a computer program. Program DIRAC1 is designed such that the user need only identify the state by specifying the quantum numbers n, l, and κ. Obviously, it would be futile to run the program for the countable infinity of cases that represent all the bound states. However, most experimental results on atomic spectra usually involve no more than the first 16 states.

The solutions of definite integrals of the class defined in (53) are available in the Maple system Version 4.3 [20, 21], and the method of solution is illustrated by the following example. Consider the Γ function which is defined by

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\, dt \qquad \text{and} \qquad z > 0. \tag{54}$$

By differentiating with respect to z m times then (54) gives

$$\int_0^{\infty} e^{-t} t^s \ln^m t \, dt = \left. \frac{\partial^m \Gamma(z)}{\partial z^m} \right]_{z=s+1} \qquad \text{and} \qquad s > -1 \tag{55}$$

which includes the class of integrals of (53) for $u = 1$. This formula can be trivially generalised for $u \neq 1$ by the variable substitution $x = ut$ into (53) whereby $\ln^m(x/u)$ can be expanded and (53) is reduced into a linear combination of definite integrals of the form (55). The latter provides a straightforward means by which one can obtain the solutions of these various definite integrals. This simple idea is by no means new. What makes this method so powerful in this application is the exploitation of Maple's very fast and efficient *diff* routine for computing partial derivatives and its support of special functions. The solutions of (53) are in terms of well-known special functions, namely the $\Gamma(z)$, $\zeta(z)$, $\psi(z)$ and $\psi(n, z)$ functions [12]. In some cases, these solutions reduce to closed form expressions. These special functions are supported by Maple via the *GAMMA*, the *Zeta*, and the *Psi* procedures.

6.2. *Indefinite Integrals*

The present version of Maple can solve indefinite integrals of the form

$$\int e^{-ut} t^i \ln^m t \, dt, \tag{56}$$

where $i = 0, 1, ...$ and $m = 0, 1$. However, in the present application the range of m must be extended to all positive integers. Furthermore, because of the presence of the "ghost" states, one needs to solve integrals of the form

$$\int e^{-ut} t^s \ln^m t Ei(ct) \, dt, \tag{57}$$

where c is a constant. Using partial integration, one generates another integrand where the function $Ei(ct)$ is replaced by its derivative and thus the integral is brought to a more solvable form. For instance, for the case $u = c = 1$, $s = 2$, and $m = 0$, the solution by partial integration is

$$\frac{t^2}{2} + 2t + 2 \ln t - (t^2 + 2t + 2) e^{-t} Ei(t). \tag{58}$$

However, for the same example but with m changed to 1, partial integration yields

$$\left(\frac{t^2}{2} + 2t + 3\right) \ln t + \ln^2 t - t + 2 \int \frac{Ei(t) e^{-t}}{t} dt - \frac{t^2}{4} - (3 + (t^2 + 2t + 2) \ln t + t) Ei(t) e^{-t}, \tag{59}$$

where it is not possible to express the remaining integral in the above in terms of the elementary functions and the exponential integral $Ei(t)$ (courtesy of Manual Bronstein). Generalising this integral becomes

$$I_1(a, b, c, d, t) = \int \frac{e^{-at} Ei(ct) \ln^d t}{t^b} \, dt, \tag{60}$$

where $d = 0, 1, 2, \ldots$. For $b = 1$, then for certain values of a and c, where $a > 0$ and $c \neq 0$, (60) cannot be solved in terms of the elementary functions and the exponential integral $Ei(ct)$. Using partial integration, solutions are obtained for (56) and (57) for $m = 0, 1, 2, \ldots$ in terms of closed form expressions and integrals of the form (60) for $b = 1$.

Although, it is not possible to solve the integrals I_1 in closed form, one can represent and manipulate them algebraically by using symbolic computation. The methodology used for telling Maple about integrals of the form (60) was to: (1) Define a Maple procedure $I1(a, b, c, d, t)$ which returns $I1(a, b, c, d, t)$ if $b = 1$ and $a > 0$. (2) Define a Maple procedure '*diff*/*I*1', such that differentiation of $I1(a, b, c, d, t)$ with respect to t returns the integrand of (60). Thus, the functionality of Maple's *diff* routine is extended to understand the integrals of (60). Indeed all symbolic computation systems allow the user to extend some aspects of the functionality of the system. The integrals $I_1(a, 1, c, d, t)$ could present a problem since they have no closed form solution. However, it turns out that, in the final computation of the particular solution of (39), all the I_1 integrals *exactly cancel out.* This cancellation also occurs for all terms involving the exponential integral. Thus, the particular solution of the jth inhomogeneous equation for the Dirac hydrogen problem is of the form

$$\sum_i \sum_k^j a_{ik} e^{-u_{ik} t} t^i \ln^k t, \tag{61}$$

where $u_{ik} > 0$. These are all examples of closed form square-integrable functions, albeit borderline cases; the integrand requiring special handling at the origin. The cancellations of all I_1 type integrals is not surprising since each of these functions is not square-integrable and should not appear in a physically meaningful solution.

6.3. *Manipulation and Simplification of Large Sums*

The program progresses iteratively through the orders as specified in (5). After the second iteration, the length and number of integrals to calculate becomes considerably larger. However, the maximum length of internal Maple objects is limited to 2^{16} computer words. This length restriction means that Maple cannot represent a sum with more than 32,767 terms in it. If the integrands are fully expanded, the total number of terms required for the calculation of the fourth iteration of the 4*s* state alone exceeds this limit.

To overcome this limitation, the expressions are regrouped in a recursive form rather than using Maple's default fully distributed form. This is done by using Maple's *collect* procedure. Just before integration, the integrand is regrouped as a multivariate polynomial in the functions of t, i.e., of the form

$$\sum_{i,j,k,l} Q_{ijkl} t^i (e^{-t/2})^j \ln^k t E_i^l(ct), \tag{62}$$

where the coefficients Q_{ijkl} are also multivariate polynomials in the mathematical constants,

$$Q_{ijkl} = \sum_{m,n,p} f_{mnp}(\alpha) \pi^m \gamma^n \zeta(2p+1), \qquad \text{where} \quad p = 1, 2, 3, \ldots$$

and the functions $f_{mnp}(\alpha)$ include irrational expressions. In this way, one is able to reduce the maximum size of the sums in the expression. The resulting expressions are simplified by causing cancellations within the various sums. These cancellations are triggered by Maple's *collect* procedure which rewrites the various expressions as univariate polynomials in t of the form

$$\textstyle\sum_i a_i t^i, \tag{63}$$

where a_i, a function of t and all the mathematical constants, is put in normal form. Not surprisingly, most of the memory and time is spent in the manipulation and simplification of these sums. These cancellations are *essential* in order to obtain the correct solutions. If these are not triggered, the program generates spurious integrals which are often non-square-integrable and "infinities" will appear in the final inner products.

Table I lists the number of definite integrals and the time (in CPU seconds) required to compute all the terms of the jth iteration on a DEC Vax 8650. These entries correspond to the total number of integrals, i.e., those integrals appearing

TABLE I

Number of Definite Integrals and the Time (in Seconds) for the jth Iteration

	$j=1$		$j=2$		$j=3$		$j=4$	
(n, l, κ)	Terms	Time	Terms	Time	Terms	Time	Terms	Time
(1, 0, 1)	18(8)	9	56(11)	35	123(15)	144	226(19)	560
(2, 0, 1)	38(12)	18	98(15)	68	193(19)	296	330(23)	1213
(2, 1, 2)	18(8)	11	56(11)	39	123(15)	167	226(19)	651
(2, 1, −1)	38(12)	16	98(15)	67	193(19)	289	330(23)	1564
(3, 0, 1)	58(16)	27	140(19)	106	263(23)	476	434(27)	2052
(4, 0, 1)	78(20)	34	182(23)	150	333(27)	742	538(31)	3342

after the integrand of each inner product has been collected according to (62). Since the calculation of the definite integrals is the longest operation beyond second order, Table I provides an overall picture of how much CPU time program DIRAC1 consumes. Another feature of Maple is its *option remember* implementation. Once an integral is computed, its solution is stored in a table and "remembered" by Maple for the remainder of the session. Consequently, an integral is computed only once and the actual number of integrals added to the "remember" table are listed in brackets with each entry in Table I. Although the total number of definite integrals is considerable and increases with each new iteration, the number of new integrals added to the "remember" table remains small and almost constant.

In spite of the massive computations, it is found that the resulting energies collapse into relatively compact closed form solutions which can be obtained by the formula in (69) (derived and discussed later) and it will be shown that the resulting expressions are correct for this particular application. Thus, the Maple program DIRAC1 is fully vindicated by this formula; the intermediate computations, no matter how numerous, are handled correctly.

The first 16 states can be calculated up to and including the fourth iteration with energies up to ninth order within a memory limit of 9 Mbytes. The smallest test run, which corresponds to the ground state, requires about 3.9 Mbytes and the largest test run, that of the 4*s* state, requires about 8.7 Mbytes. The computation of the fifth inhomogeneous equation for the 4*s* state with energies up to the 11th order required 25 Mbytes of memory and 20,118 s but this is understandable, since the intermediate computations of the $j=5$ iteration alone required the manipulation of 804 definite and 165 indefinite integrals. Nevertheless, succeeding in obtaining the energy coefficients $E_1, E_2, E_3, ..., E_{11}$, where E_{11} is of order $O(\alpha^{24})$ *in closed form* is a considerable achievement.

Program DIRAC1 is simple, yet general and computationally efficient. As a means of comparison, the program computes both the Taylor series expansion of the exact solutions for hydrogen-like systems in powers of α (as written in Eq. (1.1) of [8]), and the corresponding series expansion for the computed solution of (3). In this way, the user can verify for himself, that for a solution computed to within (and including) the jth inhomogeneous solution, the first $2j+1$ non-zero energy coefficients after ε_0 are identical. All Taylor series expansions are preformed using Maple's *taylor* routine.

7. RESULTS

7.1. *Energies*

7.1.1. *Results and Convergence*

The first-order energy E_1 as given by (20) is a function of the rest mass, the nuclear charge, the fine structure constant and the quantum numbers n and κ. In general, it is not obvious that the higher order energies can be expressed as such functions. It is found that, in fact, the energies are such functions although the complexity of the formulas increases with order. For instance, the first few energies of the first 16 states are given by (15), (19), and

$$E_2 = -R_H \frac{Z^6 A^6}{16n^6} \left\{ Z^2\alpha^2 \left(\frac{n}{|\kappa|^3} - \frac{1}{|\kappa|^2} + \frac{1}{4n^2} \right) + 4\frac{n}{|\kappa|} \left(\frac{n}{|\kappa|} - 1 \right) \left(\frac{n}{|\kappa|} + 4 \right) + 5 \right\} \quad (64)$$

$$\begin{aligned} E_3 = -R_H \frac{Z^8 A^8}{128n^8} & \left\{ Z^4\alpha^4 \left(\frac{1}{2\,|\kappa|\,n^3} - \frac{1}{4n^4} - \frac{1}{|\kappa|^4} + \frac{n}{|\kappa|^5} \right) \right. \\ & + 8Z^2\alpha^2 \left[\frac{1}{|\kappa|^2} \left(\frac{n}{|\kappa|} - 1 \right) \left(\frac{n^2}{|\kappa|^2} + 2\frac{n}{|\kappa|} - 1 \right) + \frac{1}{n^2} \left(\frac{n}{|\kappa|} - \frac{1}{2} \right) \right] \\ & \left. + 4 \left(\frac{4n^5}{|\kappa|^5} - \frac{40n^2}{|\kappa|^2} + \frac{30n}{|\kappa|} + \frac{8n^3}{|\kappa|^3} + \frac{12n^4}{|\kappa|^4} - 7 \right) \right\}. \end{aligned} \quad (65)$$

This is also true for $E_4, E_5, ..., E_{11}$, that is, as far the computations have been taken, although they are too lengthy to list here. After substituting these energies into (3) and performing a Taylor series expansion of the resulting expression in powers of α, one obtains the exact solution of the Dirac equation for hydrogen-like systems up to and including order α^{22}, given that the non-relativistic limit is the zero-order solution.

The simplicity of these final results when compared to the massive intermediate computations is enough to imply the existence of a closed form solution. This is known to be the case for this problem. It is of interest to relate this solution to the generalised solution provided by Rafelski *et al.* [22, 23] and recently cited by Vrscay [24]. The Dirac equation of (1) is modified by adding a term $\beta W(r)$ to the Hamiltonian, where $W(r)$ is a scalar potential. The term $m + W(r)$ may be interpreted as a coordinate dependent mass. Such modified Hamitonians have received much attention in the context of quark confinement [25]. Although, this system is very different than the one described in this article, its solution provides a useful general formula. For the case

$$W(r) = -\frac{\alpha_s}{r}, \qquad V(r) = -\frac{\alpha_v}{r}, \quad (66)$$

the exact energy is given by

$$\frac{E(\alpha_v, \alpha_s)}{m_0 c^2} = \frac{-\alpha_v \alpha_s + (n'+g)[(n'+g)^2 + \alpha_v^2 - \alpha_s^2]^{1/2}}{(n'+g)^2 + \alpha_v^2}, \quad (67)$$

where

$$n' = n - |\kappa|, \qquad g = (\kappa^2 + \alpha_s^2 - \alpha_v^2)^{1/2}.$$

Setting $\alpha_s = \alpha_v = Z\alpha/2$, the modified version of the Dirac Hamiltonian in (1) reduces exactly to the $\hat{H}_0$ of (2). Adding the perturbation $\hat{H}_1$ with the ordering parameter

λ to $\hat{H}_0$, the resulting formulation can again be rewritten in the form of this modified Hamiltonian, where α_v and α_s of (66) are respectively replaced by

$$\alpha'_v = \frac{Z\alpha}{2}\left(1 + \frac{\lambda}{\alpha^2}\right), \qquad \alpha'_s = \frac{Z\alpha}{2}\left(1 - \frac{\lambda}{\alpha^2}\right) \tag{68}$$

and the energy is simply $E(\alpha'_v, \alpha'_s)$ with its functional form still being given by (67). The energies $E_1, E_2, \ldots$ are given by the coefficients of the Taylor series expansion of $E(\alpha'_v, \alpha'_s)$ in powers of λ; i.e.,

$$E = \sum_{i=0}^{\infty} E_i \lambda^i, \qquad \text{where} \quad E_i = \frac{1}{i!} \frac{\partial^i E(\lambda)}{\partial \lambda^i}\bigg]_{\lambda=0}. \tag{69}$$

For $\lambda = \alpha^2$, the term $W(r)$ vanishes and $E(\alpha'_v, \alpha'_s)$ reduces to the well-known exact solution of the Dirac equation for hydrogen-like systems thus proving that Moore's perturbative solution converges towards the exact solution for this particular application.

The existence of a simple closed form formula such as $E(\alpha'_v, \alpha'_s)$ is a fortuitous result and is not always obtainable for it requires the solution of a more complicated problem than the one presented so far. The intriguing question arises: Given a series solution where each of the coefficients is in closed form (possibly a series solution obtained for the first time for a given problem) and given that enough of these coefficients are available, is it possible to infer the closed form solution whose Taylor series expansion will generate the series? This question can be answered in the affirmative for some cases, as shown by the following exercise.

7.1.2. *Series Analysis—Algebraic Function Approximant*

In this section, a method for the construction of a closed form expression from the series in powers of λ to a given order, say order $O(N)$, is presented. A Taylor series expansion of the heuristically constructed formulae in λ will simply re-generate the series to order $O(N)$. However, if the same formula can also correctly generate the series to *higher* order, one might conjecture that this constructed formula is the exact solution. Using the series solutions for the energies determined therein, the exact solution for hydrogen-like systems will be re-generated. However, it is necessary to start with some reasonable assumptions about the form of the solution.

A discussion of this method can be found in the work of Baker and Graves-Morris on the application of Padé techniques [26]. Note that the construction of a Padé approximant for a given series is a specific application of this approach, namely the special case where the function in question is a rational polynomial. For our application, one considers the more general case of what is called an *algebraic function approximant*. At this point, some reasonable and necessary properties of this function E must be assumed. Since no odd powers in α appear in any of the series solutions, it is reasonable to assume that E has the form:

$$\begin{aligned} E &= E(m_0c^2, \alpha^2, n, \langle\text{other quantum numbers?}\rangle) \\ &= m_0c^2 y(\alpha^2, n\ \langle\text{other quantum numbers?}\rangle). \end{aligned} \tag{70}$$

The Taylor series of (70) in α^2 must re-generate the first two terms of the series expansion of the exact solution for hydrogen-like atoms, namely the rest mass and the non-relativistic limit.

Assuming that the energy is a relatively simple expression involving at most square roots or roots of any shape or form, one can, without any loss of generality, [redacted] determines the closed form expression of the energy.

Let us begin with a simple form for $P(y)$, say a quadratic,

$$P(y) = \sum_{i=0}^{2} \sum_{k=0}^{2} C_{ik}\alpha^i y^k = 0, \tag{71}$$

with the understanding that all terms where the total power $i+k>2$ are not used in this trial polynomial. Consequently, $C_{22} = C_{21} = C_{12} = 0$. One then substitutes the series solution of E into (71) for any given state and collects the resulting coefficients which must all be zero, for the first few powers of α. In view of (70), all odd powers of α do not appear in the final expression for y. Thus, $C_{10} = C_{11} = 0$. The number of the remaining unknowns can always be reduced from four to three. For instance, if $C_{00} \neq 0$, then one could choose to divide both sides of (71) by C_{00} and thus without any loss of generality C_{00} can be set to either 0 or 1. An easier approach is to let C_{00} remain unknown and collect a parametric solution at the end. Either way, one only needs three equations to solve for the coefficients C_{ik}. After the rest mass and nonrelativistic limit, only the energy to first order is required to construct the polynomial.

Using one of the procedures of the Maple program AFA (algebraic function approximant), one obtains a parametric solution in C_{20} for the ground state:

$$C_{00} = -C_{20}, \qquad C_{01} = 0, \qquad C_{02} = C_{20}. \tag{72}$$

The term C_{20} is reduced to a scaling factor for the polynomial $P(y)$. Hence, if $C_{20} \neq 0$, one of the roots of $P(y)$ gives the exact solution for hydrogen-like atoms in the case where $n = |\kappa| = 1$. Furthermore, the quadratic expression in (71) also yields the correct energy formula in agreement with the exact solution for all cases, where $n = |\kappa|$, namely:

$$C_{00} = -C_{20}\kappa^2, \qquad C_{01} = 0, \qquad C_{02} = C_{20}\kappa^2. \tag{73}$$

The remaining case of $n \neq \kappa$ is more complicated and requires a fourth-order polynomial and consequently more equations. However, in view of the fact that one has both matter and anti-matter solutions, one expects a solution of the form $y^2 = f(\alpha^2, n, \ldots)$ and this eliminates all odd terms in y from the polynomial, which is given by

$$P(y) = \sum_{i=0}^{2} \sum_{k=0}^{2} C_{(2i)(2k)}\alpha^{2i} y^{2j} = 0. \tag{74}$$

Terms where $i+k>6$ are excluded and hence $C_{44}=0$. For instance, in the case $n=4$ and $|\kappa|=1$, Maple yields a parametric solution in C_{40},

$$\begin{gathered} C_{42}=0, \qquad C_{00}=C_{04}=64C_{40}, \qquad C_{20}=16C_{40} \\ C_{02}=-128C_{40}, \qquad C_{22}=-52C_{40}, \qquad C_{24}=36C_{40} \end{gathered} \tag{75}$$

and one of the roots of (74) yields the correct solution in agreement with the exact solution. The solutions presented above were all generated via the second procedure of program AFA. In the case above, one needs seven equations and thus the energies $E_1, E_2, ..., E_5$ to construct the series. Since program DIRAC1 obtains the energies to at least ninth order for the first 16 states, this provides enough terms to "infer" the closed form solution and at least four more to verify it.

Thus, in general, one can now reconstruct possible closed form solutions from the series coefficients for all states. Of course, in this example, one already had the closed form solution but this exercise demonstrates that this approach is a viable alternative if one has only an algebraic series solution for a given problem.

7.2. *Matrix Elements*

Since the Maple system provides a means of generating the exact solution of the wave-function to high-order, one can algebraically calculate matrix elements to an order higher than ever obtained before.

7.2.1. *Matrix elements for the Stark Effect*

The first physical interaction considered is the simple matrix element that gives rise to the Stark effect and to electric-dipole transitions. Note that the dimensionless parameter t defined in (12) depends on the quantum number n for each state. To calculate this matrix element which involves the mixing of states, one has to rewrite the parameter t of each state in terms of some common variable such as r and the calculations become rapidly cumbersome. Such an example emphasizes how the Maple system can provide a rapid and efficient means of calculation.

Following the analysis in Section 3 of [5], this matrix element is written according to Eq. (3.5) of [10] as

$$(\Phi_{n'l'm'\kappa'}|\, H_\xi \,|\Phi_{nlm\kappa})/q\xi a_0 = -\tfrac{1}{2}A_{n'l'\kappa'}A_{nl\kappa}B^{nl\kappa}_{n'l'\kappa'}A^{nl\kappa}_{n'l'\kappa'}. \tag{76}$$

Here $A_{nl\kappa}$ is the normalising constant given by Eq. (2.19) of [5], and $A^{nl\kappa}_{n'l'\kappa'}$ is the angular integral that gives the standard selection rules and is defined by Eq. (3.6) of [10]. Finally,

$$B^{nl_k}_{n'l'\kappa'} = \langle R_{1_{n}'l'\kappa'}|r|R_{1_{n}l\kappa}\rangle + \langle R_{2_{n}'l'\kappa'}|r|R_{2_{nl\kappa}}\rangle \tag{77}$$

is the radial integral that separates out. All of these integrals are straightforward to evaluate with the Maple system, and hence the total matrix element in (76) can be written as a power series in α^2. From the output of program DIRAC1, these matrix elements can be computed to high-order in α^2 using a simple Maple program called STARK. For example, for the $1s_{1/2} \rightarrow 2p_{3/2}$ transition, the matrix element to order $O(\alpha^6)$ is given by

$$\alpha^0: \frac{256}{243\sqrt{3}}$$

$$\alpha^2: \frac{192\ln(27/32) - 248}{729\sqrt{3}}$$

$$\alpha^4: \frac{1}{5832\sqrt{2}}(4800\ln(2)^2 - 235 - 5760\ln(2)\ln(3) \\ + 848\ln(2) + 1728\ln(3)^2 - 624\ln(3) - 32\pi^2).$$

The exact α^0 and α^2 coefficients of the matrix elements for a number of transitions is given in Table II. The α^0 term is just the well-known nonrelativistic result [3]. When reference [10] was written, there did not seem to exist an exact calculation of the α^2 coefficient in general. Only the α^0 and α^2 coefficients of (78) were calculated manually. When the exact answers of Table II are compared with the numerical results of Table 4 of [10], one sees that the numerical methods used for that earlier paper are fairly accurate. The α^2 coefficient differs from the exact answer in the sixth decimal place only for most values; the worst case differing in the fifth digit for the transition $2p_{1/2} \rightarrow 3s_{1/2}$. It has been verified that the Maple program STARK vindicates all the numerical results presented in Table 4 of that earlier work (note the omission of a minus sign in the heading of Table 4—the correct heading is given in Table II).

7.2.2. *Matrix Elements for the Hyperfine Interaction*

The second physical interaction considered is the matrix element required for the hyperfine splitting. There is no mixing of states in this case and thus the calculations are much easier.

Following the analysis in [6], the matrix elements are defined in [10, Eq. (3.8)] and give the hyperfine splitting as

$$\Delta E = q g_N \mu_N \left[\frac{I+J}{J}\right]\left[\frac{4\kappa}{2|\kappa|+1}\right] A^2 B_{nl\kappa}, \tag{79}$$

where $J = |\kappa| - \frac{1}{2}$, A^2 is the normalisation constant defined in (18) and $B_{nl\kappa}$ is a radial integral, namely,

$$B_{nl\kappa} = \mathrm{Im}\left\langle R_2 \left|\frac{1}{r^2}\right| R_1 \right\rangle, \tag{80}$$

where the Im indicates that the imaginary part of the integral is evaluated. One can

TABLE II

Coefficients of $-(\Phi_{n'l'm'\kappa'}\,|\,H_\xi\,|\,\Phi_{nlm\kappa})/q\xi a_0$

States		Actual values		Floating point	
$nlm\,\kappa$	$n'l'm'\kappa'$	α^0	α^2	α^0	α^2
1001	2102	$\frac{256}{243\sqrt{3}}$	$\frac{192\ln(27/32)-248}{729\sqrt{3}}$	0.6082373206	−0.2222447018
	310−1	$\frac{27}{64\sqrt{6}}$	$\frac{108\ln(4/3)-153}{512\sqrt{6}}$	0.1722297475	−0.0972223658
2001	3102	$\frac{27648\sqrt{2}}{15625\sqrt{3}}$	$\frac{69120\ln(125/144)-214848}{78125\sqrt{6}}$	1.4447678380	−1.1738135117
	210−1	$-\frac{3}{\sqrt{3}}$	$\frac{5}{4\sqrt{3}}$	−1.7320508076	0.7216878365
210−1	320−2	$\frac{55296\sqrt{2}}{15625\sqrt{5}}$	$\frac{138240\ln(125/144)-265728}{78125\sqrt{10}}$	2.2382247104	−1.1547682733
	3001	$\frac{6912}{15625\sqrt{2}}$	$\frac{17280\ln(25/24)-6168}{78125\sqrt{2}}$	0.3128014126	−0.0494417744
2102	320−2	$\frac{55296}{78125\sqrt{5}}$	$\frac{69120\ln(25/24)-40128}{390625\sqrt{5}}$	0.3165327741	−0.0427108403
	3001	$\frac{6912}{15625}$	$\frac{49704}{78125}+\frac{1728\ln(125/96)}{15625}$	0.4423680000	0.6654036776
	3203	$\frac{165888\sqrt{6}}{78125\sqrt{5}}$	$\frac{414720\ln(3125/3456)-473472}{390625\sqrt{30}}$	2.3260313503	−0.2408109698
	420−1	$\frac{4096}{6561\sqrt{30}}$	$\frac{5120\ln(9/8)-5664}{32805\sqrt{30}}$	0.1139801654	−0.0281664070

now obtain the matrix elements as a series in α^2 using the Maple system. In the earlier work of [10, Eq. (3.10)], (80) was rewritten as

$$A^2\,B_{nl\kappa}=\frac{\hbar}{2m_0c}\,\frac{2}{a_0^3}\,B^B_{ln\,\kappa}\,[1+\alpha^2\,C_{ln\,\kappa}+\alpha^4 D_{nl\,\kappa}+\cdots], \tag{81}$$

where the coefficients $B^0_{nl\,\kappa}$ and $C_{nl\,\kappa}$ where evaluated numerically for a number of states. At that time, the exact analytic values for all the $B^0_{nl\,\kappa}$ and for only a few of the $C_{nl\,\kappa}$ were known [3, 6, p. 180]. For the remaining values of $C_{nl\,\kappa}$, the rational fractions that reproduced the numerical $C_{nl\,\kappa}$'s to within 3 in the sixth significant figure were computed and presented in Table 5 of that earlier work. The exactness of the remaining fractions had yet to be verified.

Using a Maple program called HYPERFINE, it is now possible to generate such [illegible] The first three terms of the series in (81) for the ground state $[(n, l, \kappa) = (1, 0, 1)]$ are, respectively,

$$B^0_{nl\,\kappa} = 1, \qquad C_{nl\,k} = \tfrac{3}{2}, \qquad D_{nl\,\kappa} = \tfrac{17}{8}. \tag{82}$$

For the (3, 2, −2) state, these are

$$B^0_{nl\,\kappa} = -\tfrac{1}{270}, \qquad C_{nl\,\kappa} = \tfrac{433}{1080}, \qquad D_{nl\,\kappa} = \tfrac{33737}{259200} \tag{83}$$

and, for the (4, 3, −3) state, these are

$$B^0_{nl\,\kappa} = -\tfrac{1}{1344}, \qquad C_{nl\,\kappa} = \tfrac{1649}{10080}, \qquad D_{nl\,\kappa} = \tfrac{1498447}{67737600}. \tag{84}$$

In general, it is found that this program exactly reproduces all the rational fractions that were inferred in Table 5 of [6] and it would be redundant to reproduce this table here. Thus, the Maple system provides further vindication of the numerical work in that earlier paper.

8. Applications to Other Systems

Although the exact solution to the hydrogen-like atom can be found, this is certainly not the case for other atomic systems. The separation of $\hat{H}$ into $\hat{H}_0$ and $\hat{H}_1$ and the reduction to the two component equation is independent of the form of the potential and hence is valid for any general potential $V(r)$. Much of what has been presented so far remains applicable. However, although (9) can be solved numerically for atomic systems, difficulties may occur due to the quadratic energy dependence or from more complicated potentials. Any of the above possible problems have been circumvented by solving (9) by perturbation theory. This has been discussed by Moore as early as 1975 [4, 8] and demonstrated at length more recently [10].

This procedure has also been applied successfully to more complex systems, namely, atomic systems in the alkali system sequence. The non-relativistic solutions are derived from a self-consistent Hartree–Fock calculation. Since one deals with closed shells for all the inner electrons, one can model the problem with an effective central potential $V(r)$ and consequently Moore's procedure is applicable. The range of application extends from the lithium atomic system to systems as heavy as radium II (fracium sequence) which represents a very broad range of light and heavy nuclei. These applications and their results are the subject a forthcoming article.

9. Conclusions

In this paper, it has been shown that Moore's decoupling technique is a useful method in obtaining approximate solutions to the one-particle Dirac equation. In principle, these solutions can be obtained to within *any* order in the perturbation parameter λ. This was demonstrated via the approach of "ghost" states for solving the various inhomogeneous equations that appear in the hierarchy of perturbative equations. All resulting computations were rendered feasible by the Maple system. Once the wavefunction was solved for a number of states, it was also shown that the Maple system provided an excellent means of calculating matrix elements to any order in λ using two examples, namely the hyperfine interaction matrix element and the simple dipole matrix element. The resulting programs are compact and efficient.

In practice, one desires the energy expansion to high order, either as a means of "summing" the series beyond its radius of convergence using Padé techniques or some other method which can handle divergent series, or, as a means of inferring possible closed form solutions to the problem (as demonstrated in this work). One usually does not want the wave function beyond the first few orders. Albeit the method presented solves the energies to order $O(\lambda^{2j+1})$ and only requires the solution of the wave function to order $O(\lambda^{j})$, the calculation of energies to very high order requires a number of computations that appears to grow exponentially in j. Unless one is solving a new problem for the first time or one has no other alternative, this method is not recommended beyond the solution of the fifth iteration. For energy calculations to higher order, one could consider the technique recently devised for perturbed Dirac equations [24]. This method involves a useful synthesis of the relativistic hypervirial (HV) and Hellmann–Feynman (HF) theorems to construct expansions for eigenvalues of perturbed radial Dirac equations to arbitrary order. The HVHF method is simple and flexible, requiring no matrix elements. Only the unperturbed energy is required as input. It solves for the perturbed eigenenergies without ever having to solve for the wavefunction itself. Such a method would provide an ideal complement to the one presented in this article whenever its application is possible. However, in some applications, the method in its present form also requires the use of symbolic computation.

From this point, this project could proceed in different directions. For instance, one can contemplate the solution of perturbative equations via the use of "ghost" states for a class of non-relativistic or relativistic quantum mechanical problems. At the present stage of development, this class is restricted to separable problems, yet not solvable in closed form.

Another project which is currently under investigation is the generalisation of this work to the relativistic 2-body problem, such as the Breit Interaction [27, 28]. Although this problem is separable in the center of momentum frame, there has yet to be found a closed form solution for this type of problem. This is exactly the type of problem this technique was designed to tackle.

Although separability is possible in some problems, this is not the case for many-particle systems where the perturbation involves the two-particles interactions of the form $1/r_{12}$. This type of problem was not examined in this article. However, in view of the results of this present work, even in the worst possible scenario where one must resort to formal solutions in terms of a basis set, there is the intriguing possibility that symbolic computation may yet prove a useful means of obtaining algebraic solutions to such problems.

Simple closed form solutions do not exist for most present physical theories. However, the approach presented in this work may be a useful tool in pushing present theories to the next decimal or the next order of complexity [29]. One now has to contemplate the representation of wavefunctions by rational approximants or continued fractions often because the perturbative methods yield either divergent series or solutions which cannot be expressed in a straightforward way. Such representations are often unwieldy to manipulate by hand.

Symbolic computation presents a viable alternative for the manipulation, calculation, and storage of the required objects and it also represents the next level beyond the digital calculator as the extension of the human mind. One may be so bold as to anticipate that, in the future of theoretical physics, symbolic computation will be widely used, not as a result of extravagance or even preference but as a result of necessity.

APPENDIX

In this Appendix, the energy formulas given by (48) to (50), which minimise the information needed about the wave-function, are derived. It is assumed that both $\hat{H}_0$ and $\hat{H}_1$ are hermitian. Starting from (5),

$$(\hat{H}_0 - E_0)|\Phi^l\rangle = -\hat{H}_1\,|\Phi^{l-1}\rangle + \sum_{i=1}^{l} E_i\,|\Phi^{l-i}\rangle \tag{A.1}$$

and taking the inner product of $\langle\Phi^k|$ with (A.1) gives

$$\langle\Phi^k|\,\hat{H}_0 - E_0\,|\Phi^l\rangle = -\langle\Phi^k|\,\hat{H}_1\,|\Phi^{l-1}\rangle + \sum_{i=1}^{l} E_i\langle\Phi^k|\Phi^{l-i}\rangle. \tag{A.2}$$

For the remainder of this section, the inner products $\langle\Phi^a|\Phi^b\rangle$ are replaced by the notation M_a^b, as defined in (32). Taking the adjoint of (A.1), replacing l with k, substituting this result into (A.2) with l replaced by $l-1$, results in

$$\langle\Phi^{k-1}|\,\hat{H}_1\,|\Phi^{l-1}\rangle = \langle\Phi^k|\,\hat{H}_1\,|\Phi^{l-2}\rangle + \sum_{i=1}^{k} E_i M_{k-i}^{l-1} - \sum_{i=1}^{l-1} E_i M_k^{l-i-1}. \tag{A.3}$$

Now, when $k=1$ and $l=j$,

$$\langle\Phi^0|\,\hat{H}_1\,|\Phi^{j-1}\rangle = \langle\Phi^1|\,\hat{H}_1\,|\Phi^{j-2}\rangle + M_0^{j-1} - \sum_{i=1}^{j-1} E_i M_1^{j-i-1} \tag{A.4}$$

and, similarly, when $k=2$ and $l=j-1$,

$$\langle\Phi^1|\,\hat{H}_1\,|\Phi^{j-2}\rangle = \langle\Phi^2|\,\hat{H}_1\,|\Phi^{j-3}\rangle + \sum_{i=1}^{2} E_i M_{2-i}^{j-2} - \sum_{i=1}^{j-2} E_i M_2^{j-i-2}. \tag{A.5}$$

Substituting (A.5) into (A.4) gives $\langle \Phi^0 | \hat{H}_1 | \Phi^{j-1} \rangle$ in terms of $\langle \Phi^2 | \hat{H}_1 | \Phi^{j-3} \rangle$. Thus, as k is incremented while l is decremented, by recursive substitution, one constructs a formula that reduces the matrix element in $\langle \Phi^0 | \hat{H}_1 | \Phi^{l-1} \rangle$ to

$$\langle \Phi^0 | \hat{H}_1 | \Phi^{l-1} \rangle = \langle \Phi^k | \hat{H}_1 | \Phi^{l-(k+1)} \rangle + \sum_{j=1}^{k} \sum_{i=1}^{j} E_i M_{j-i}^{l-j} - \sum_{j=1}^{k} \sum_{i=1}^{l-j} E_i M_j^{l-j-i}. \tag{A.6}$$

Even Case

In order to generate (48), set $l = 2p$ ($p = 1, 2, \ldots$), and $k = p - 1$, (A.6) becomes

$$\langle \Phi^0 | \hat{H}_1 | \Phi^{2p-1} \rangle = \langle \Phi^{p-1} | \hat{H}_1 | \Phi^p \rangle + \sum_{j=1}^{p-1} \sum_{i=1}^{j} E_i M_{j-i}^{2p-j} - \sum_{j=1}^{p-1} \sum_{i=1}^{2p-j} E_i M_j^{2p-j-i}. \tag{A.7}$$

The first double summation on the right can be rewritten as ($p \geqslant 2$)

$$\sum_{j=1}^{p-1} \sum_{i=1}^{j} E_i M_{j-i}^{2p-j} = \sum_{j=2}^{p-1} \sum_{i=1}^{j-1} E_i M_{j-i}^{2p-j} + \sum_{j=1}^{p-1} E_j M_0^{2p-j}. \tag{A.8}$$

Defining $m = 2p - j$, the double summation on the right can be rewritten as, with M_a^b real,

$$\sum_{j=2}^{p-j} \sum_{i=1}^{j-1} E_i M_{j-i}^{2p-j} = \sum_{m=p+1}^{2p-2} \sum_{i=1}^{2p-m-1} E_i M_m^{2p-i-m} \tag{A.9}$$

and, since m is only a dummy variable, it can be replaced by j. Similarly, the second summation in (A.7) can be decomposed into

$$\sum_{j=1}^{p-1} \sum_{i=1}^{2p-j} E_i M_j^{2p-i-j} = \sum_{j=1}^{p-1} \sum_{i=1}^{2p-j-1} E_i M_j^{2p-j-i} + \sum_{m=p+1}^{2p-1} E_m M_0^{2p-m} \tag{A.10}$$

and the dummy variable m can be replaced by i. Next, using the identity,

$$\sum_{j=1}^{p-2} \sum_{i=1}^{p-j-1} E_i M_j^{2p-j-i} = \sum_{j=p+1}^{2p-2} \sum_{i=1}^{2p-j-1} E_i M_j^{2p-j-i}. \tag{A.11}$$

The proof of (A.11) is as follows: Rewrite the left-hand side as

$$\sum_{j=1}^{p-2} \sum_{i=1}^{p-j-1} E_i M_j^{2p-j-i} = \sum_{i=1}^{p-2} E_i \sum_{j=1}^{p-i-1} M_j^{2p-j-i}. \tag{A.12}$$

This identity follows by comparing the sums term by term. Next, by defining $j' = j - p$, the right-hand side of (A.11) can also be rewritten as

$$\sum_{j=p+1}^{2p-2} \sum_{i=1}^{2p-j-1} E_i M_j^{2p-j-i} = \sum_{j'=1}^{p-2} \sum_{i=1}^{p-j'-1} E_i M_{j'+p}^{p-j'-i}, \tag{A.13}$$

which, as for (A.12) and chopping the prime, becomes

$$\sum_{j=p+1}^{2p-2} \sum_{i=1}^{2p-j-1} E_i M_j^{2p-j-i} = \sum_{i=1}^{p-2} E_i \sum_{j=1}^{p-i-1} M_{j+p}^{p-j-i}. \tag{A.14}$$

Comparing (A.14) with (A.12), (A.11) is established if

$$\sum_{j=1}^{p-i-1} M_j^{2p-i-j} = \sum_{k=1}^{p-i-1} M_{k+p}^{p-k-i}.$$

This can be readily seen by setting $j' = p - k - i$ on the right side of the above and then dropping the prime.

Combining (A.8) to (A.11) into (A.7), and after some rearranging of terms, Eq. (33) of the conventional energy formula becomes

$$E_{2p} = \langle \Phi^{p-1} |\, \hat{H}_1 \,| \Phi^p \rangle - E_p M_0^p - 2 \sum_{i=p+1}^{2p-1} E_i M_0^{2p-i} - \sum_{j=1}^{p-1} \sum_{i=p-j}^{2p-j-1} E_i M_j^{2p-i-j}. \tag{A.15}$$

This formula only requires the knowledge of the wavefunction to order p. The double summation in (A.15) can be exactly rewritten as

$$\sum_{j=1}^{p-1} \sum_{i=p-j}^{2p-j-1} E_i M_j^{2p-j-i} = \sum_{j=1}^{p-1} E_j \sum_{i=1}^{j} M_{p-i}^{p+i-j} + \sum_{j=p}^{2p-2} E_j \sum_{i=1}^{2p-j-1} M_i^{2p-i-j}. \tag{A.16}$$

Again, the proof of this identity is similar to that of (A.12). Substitution of this identity into (A.15) and some term rearranging yields

$$E_{2p} = \langle \Phi^{p-1} |\, \hat{H}_1 \,| \Phi^p \rangle - \sum_{j=1}^{p-1} E_j \sum_{i=1}^{j} M_{p-i}^{p+i-j} - E_{2p-1} M_0^1 - \sum_{i=p+1}^{2p-1} E_i M_0^{2p-i} - \sum_{i=p}^{2p-2} E_i \sum_{j=0}^{2p-i-1} M_j^{2p-i-j}. \tag{A.17}$$

The sum inside the double summation above can be decomposed as

$$\sum_{j=0}^{2p-i-1} M_j^{2p-i-j} = \sum_{j=0}^{2p-i} M_j^{2p-i-j} - M_{2p-i}^0. \tag{A.18}$$

The summation on the right is identically zero by virtue of the orthogonality conditions expressed in (31). Thus, the number of terms in (A.16) is almost halved. This illustrates the full exploitation of the orthogonality conditions and (A.17) becomes (48).

Odd Case

The proof for the odd case of (49) proceeds in complete analogy with the above. A further reduction on Eq. (49) can be obtained by exploiting the commutativity of real inner products involved in the orthogonality equations. This reduction creates a further subdivision of the odd case in (49) into even and odd cases.

Thus, for $m = 2k$, where $k = 1, 2, 3, \ldots$,

$$\sum_{j=0}^{2k} M_j^{2k-j} = 2 \sum_{j=0}^{k-1} M_j^{2k-j} + M_k^k = 0 \tag{A.19}$$

and, for $m = 2k + 1$, where $k = 0, 1, 2, \ldots$,

$$\sum_{j=0}^{2k+1} M_j^{2k+1-j} = 2 \sum_{j=0}^{k} M_j^{2k+1-j} = 0. \tag{A.20}$$

Using both (A.19) and (A.20), Eq. (49) becomes (50).

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