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Hydrogen Atom in a Finite Linear Space[1]

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A Galerkin-collocation-type technique for solving numerically differential boundary value problems was developed several years ago. Such a method is based on a certain finite-dimensional matrix representation of the derivative d/dx obtained through Lagrange's interpolation. Recently, an extension to separable multivariate problems has been given; in this context, the authors have found a matrix representation of the quantum angular momentum, yielding the precise eigenvalues and finite-dimensional vectors that coincide exactly with the spherical harmonics evaluated at a certain set of points. The aim of this paper is to give additional properties of such a matrix representation and to show how these findings can be applied to obtain binding energies and eigenfunctions for the hydrogen atom. We consider three cases: the Coulomb potential, the fine-structure splitting, and the hydrogen atom in a uniform magnetic field. Since this last case is a nonseparable problem in the coordinates, the method requires a modification that is introduced in this paper.

Key Words: hydrogen atom; eigenvalue problem; angular momentum; numeric partial differentiation; boundary value problems.

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1. INTRODUCTION

Recently, the authors have found a finite-dimensional version of the eigenproblem of the quantum angular momentum that yields the exact eigenvalues and finite-dimensional vectors coinciding exactly with the spherical harmonics evaluated at a certain set of points [9]. The matrix associated to the square of the angular momentum L of a system described by three classical degrees of freedom is obtained by using a certain $N \times N$ (N odd) matrix representing an angular derivative in the space of trigonometric polynomials of degree at

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most $(N-1)/2$ which has the generic form

$$D_t = Q\tilde{D}_t Q^{-1},$$

$$(\tilde{D}_t)_{ij} = \begin{cases} \sum_{l=1}^{\prime N} \frac{1}{2}\cot\frac{(t_i - t_l)}{2}, i = j, \\ \frac{1}{2}\csc\frac{(t_i - t_j)}{2}, i \neq j, \end{cases} \qquad Q_{ij} = q'(t_i)\delta_{ij}, i, j = 1, \dots, N, \tag{1}$$

where $q'(t)$ is the derivative of the trigonometric polynomial $q(t) = \Pi_{l=1}^{N}\sin[(t - t_l)/2]$, and the set of nodes t_j is any set of different points of $[-\pi, \pi]$. Hereafter, a prime appended to a sum sign excludes the divergent term.

The finite-dimensional representation of L^2 is given by

$$\mathbf{L}^2 = -\left[\mathbf{D}_\theta^2 + \cot\boldsymbol{\Theta}\mathbf{D}_\theta + \sin^{-2}\boldsymbol{\Theta}\mathbf{D}_\varphi^2\right], \tag{2}$$

where

$$\mathbf{D}_\theta = 1_M \otimes D_\theta, \qquad \mathbf{D}_\varphi = D_\varphi \otimes 1_K, \qquad \boldsymbol{\Theta} = 1_M \otimes \Theta. \tag{3}$$

Here, 1_M and 1_K are identity matrices of dimension M and K, respectively; and D_θ and D_φ are matrix representations of the derivatives $d/d\theta$ and $d/d\varphi$ in the subspaces S_θ and S_φ of trigonometric polynomials of degrees at most $(K-1)/2$ and $(M-1)/2$, respectively. Θ is a diagonal matrix with entries $(\Theta)_{jk} = \theta_j\delta_{jk}$ and the nodes θ_j are restricted to be in $[0, \pi]$. If $M \geq K$, the eigenvalue problem of (2),

$$\mathbf{L}^2\mathbf{y}_s = \lambda_s\mathbf{y}_s,$$

reproduces exactly the first $(K+1)^2/4$ eigenvalues and determines the corresponding spherical harmonics $Y_l^m(\theta, \varphi)$ at the nodes (θ_j, φ_k), save for a constant factor, and ordered as

$$\lambda_s = l(l+1),$$

where

$$s = l^2 + l + m + 1, \qquad l = 0, 1, \dots, (K-1)/2, \qquad m = -l, \dots, l.$$

The components y_{rs} of $\mathbf{y}_s$ are given by

$$y_{rs} = c_{lm}P_l^m(\theta_j)e^{im\varphi_k},$$

where c_{lm} is a normalization constant and

$$r = j + (k-1)K, \qquad j = 1, 2, \dots, K, \qquad k = 1, 2, \dots, M.$$

In order to have a positive semidefinite matrix $\mathbf{L}^2$, the φ-nodes must be given by $\varphi_k = -\pi + 2\pi k/M$, $k = 1, 2, \dots, M$, and the θ-nodes must satisfy the condition

$$\sum_{l=1}^{K}{}' \cot\frac{(\theta_j - \theta_l)}{2} = -\cot(\theta_j). \tag{4}$$

It is also possible to combine D_φ, as given by (1), and the matrix representation of $d/d\theta$

given in [4] into (3) to yield equivalent results [9]. The way in which the matrix (1) is obtained is similar to the way in which the finite-dimensional matrix representation D_x of d/dx, which has been used to solve two-point boundary value problems [2, 5, 8], was obtained. Such a matrix is given by

$$D_x = P\tilde{D}_x P^{-1},$$

$$(\tilde{D}_x)_{ij} = \begin{cases} \sum_{l=1}^{\prime\, N} \frac{1}{(x_i - x_l)}, i = j, \\ \frac{1}{(x_i - x_j)}, i \neq j, \end{cases} \qquad P_{ij} = p'(x_i)\delta_{ij}, i, j = 1, 2, \ldots, N. \tag{5}$$

Here, $p(x) = \Pi_{l=1}^{N}(x - x_l)$, and the set of nodes x_j are chosen by imposing the condition

$$\sum_{l=1}^{N}{}' \frac{1}{(x_j - x_l)} = -\frac{\gamma'(x_j)}{\gamma(x_j)}, \qquad j = 1, 2, \ldots, N, \tag{6}$$

where $\gamma(x)$ is a function defined by the boundary conditions and the differential equation (see [7, 8]).

The purpose of this paper is to give an application of the finite-dimensional representation of the angular momentum and the angular derivatives. We incorporate such matrices in the numerical technique used to solve multidimensional boundary value problems [6] and choose as trial examples the following eigenvalue problems: the hydrogen atom, the fine-structure splitting, and the hydrogen atom in a uniform magnetic field. Since the last case is a nonseparable problem in the coordinates for an intense field, i.e., the solution cannot be written as a (tensor) product of univariate functions, a modification of the method will be introduced.

2. THE HYDROGEN ATOM

In this and in the next sections, the units of length and energy will be taken as the Bohr radius $a_0 = \hbar^2/m_e e^2 = 5.3 \times 10^{-9}$ cm and two times a Rydberg $m_e e^4/\hbar^2 = 27.2$ eV, respectively.

To obtain an appropriate matrix form of the Schrödinger equation for the electron in a Coulomb field

$$\left[-\frac{1}{2r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{2r^2}L^2 - \frac{1}{r}\right]\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi), \tag{7}$$

it is necessary to extract from $\psi(r,\theta,\varphi)$ the singular behavior at the endpoints of the intervals (see [2, 7, 8]). This can be done in part through the change of variable

$$\psi(r,\theta,\varphi) = \psi_\infty(r,\theta,\varphi) f(r,\theta,\varphi), \tag{8}$$

where $\psi_\infty(r,\theta,\varphi)$ is the solution of (7) for bound states when $r \to \infty$, given by

$$\psi_\infty(r,\theta,\varphi) = e^{-\sqrt{2\varepsilon}r}. \tag{9}$$

The unknown energy is written here as $-\varepsilon$ because it will be used in the numerical calculations as a trial parameter.

The substitution of (8) and (9) in (7) yields

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial r^2}-\left(\frac{1}{r}-\sqrt{2\varepsilon}\right)\frac{\partial}{\partial r}+\frac{1}{2r^2}L^2-\left(\frac{1-\sqrt{2\varepsilon}}{r}\right)-\varepsilon\right]f(r,\theta,\varphi)=Ef(r,\theta,\varphi). \quad (10)$$

Since $f(r,\theta,\varphi)$ can be written as a product of univariate functions of r, θ, and φ, we can project each of these functions on subspaces of polynomials to yield finite-dimensional matrix representations of the partial derivatives [9]. Thus, to the projection of the angular variables described above, we add the projection of the radial function on a subspace of polynomials S_r depending on r of degree at most $N-1$. This yields a tensor projection space $S=S_\varphi\otimes S_\theta\otimes S_r$ of dimension $\tilde{N}=MKN$ in which the matrix form of (10) is given by

$$\mathbf{H}\mathbf{f}_s=E_s\mathbf{f}_s,\qquad s=1,2,\ldots,\tilde{N}, \quad (11)$$

where the discretized Hamiltonian is given by

$$\mathbf{H}=-\frac{1}{2}\mathbf{D}_r^2-(\mathbf{r}^{-1}-\sqrt{2\varepsilon}\mathbf{1})\mathbf{D}_r+\frac{1}{2}\mathbf{r}^{-2}\mathbf{L}^2-(1-\sqrt{2\varepsilon})\mathbf{r}^{-1}-\varepsilon\mathbf{1}. \quad (12)$$

Here, $\mathbf{D}_r$ is the tensor product

$$\mathbf{D}_r=1_M\otimes 1_K\otimes D_r,$$

where D_r is the representation of the radial derivative having the structure of (5), the diagonal matrix $\mathbf{r}$ is defined by

$$\mathbf{r}=1_M\otimes 1_K\otimes R,$$

and the nonzero entries of R are the radial nodes r_j, $j=1,2,\ldots,N$. $\mathbf{L}^2$ is given by (2), and $\mathbf{1}$ is the identity matrix of dimension $\tilde{N}$. Since the part of $f(r,\theta,\varphi)$ depending on r consists of polynomials (Laguerre polynomials multiplied by a power of r) and the dimension of D_r is N, one would expect a set of N times $(K+1)^2/4$ eigenvectors $\mathbf{f}_s$ coinciding exactly with the first eigenfunctions of the hydrogen atom evaluated at the nodes (provided $M\geq K$). However, due to the fact that the argument of the radial functions depends on the principal quantum number n, which is related to the index defining the degree n_L of certain Laguerre polynomial and to the azimuthal quantum number l through $n=n_L+l+1$, the projection of the radial part of (12) for the s-states on S_r, i.e., the eigenvalue equation

$$H_r f_j=E_j f_j,\qquad j=1,2,\ldots,N,$$

with

$$H_r=-\frac{1}{2}D_r^2-(R^{-1}-\sqrt{2\varepsilon}1_N)D_r-(1-\sqrt{2\varepsilon})R^{-1}-\varepsilon 1_N, \quad (13)$$

will reproduce only one exact eigenvalue: the one corresponding to the case in which $\varepsilon=-E=1/(2n^2)$ for some $n\leq N$. As a consequence, the number of exact energies yielded by (11) is given by the known formula

$$\sum_{l=0}^{n-1}(2l+1)=n^2,$$

for some $n \le n_{\max}$, provided $\varepsilon = 1/(2n^2)$. Since D_r yields exact derivatives of polynomials of degree at most $N-1$ and the radial part of $f(r, \theta, \varphi)$ is a polynomial of degree $n-1 = n_L + l$, we have again that $n_{\max} = N$, and therefore, the method yields the correct number of exact eigenvalues corresponding to the multiplet defined by n provided $n \le N$ and $M \ge K \ge 2N - 1$. It is necessary, however, to choose the radial nodes in such a form that [7]

$$\sum_{l=1}^{N}{}' \frac{1}{(r_j - r_l)} = \sqrt{2\varepsilon} - \frac{1}{r_j}, \qquad j = 1, 2, \ldots, N, \tag{14}$$

in order to look for a well-behaved solution at $r = 0$. Therefore these points coincide with the N zeros of the Laguerre polynomial $L_N^{(1)}(2\sqrt{2\varepsilon}r)$ and yield a positive definite matrix $\mathbf{r}^{-1}$ in (12) and a Hermitian matrix H_r (save for a similarity transformation). The first assertion is obvious, and the latter can be shown by setting the main diagonal of D_r apart by writing $D_r = PDP^{-1} + d$, $d_{jk} = (D_r)_{jj}\delta_{jk}$, and using (14) to obtain

$$H_r = P\left[\frac{1}{2}(-D^2 + dD - Dd + d^2) + V\right]P^{-1} = P\left(\frac{1}{2}D_r^t D_r + V\right)P^{-1},$$

where V is the diagonal matrix

$$V = -(1 - \sqrt{2\varepsilon})R^{-1} - \varepsilon 1_N.$$

Therefore, the radial part $\mathbf{H}_r$ of (12) also has real eigenvalues because

$$\mathbf{H}_r = 1_M \otimes 1_K \otimes H_r.$$

However, because of the arbitrariness of the θ-nodes, some complex eigenvalues can be found in the spectrum of (11). To exclude them we can fix the θ-nodes through the condition (4) to give a positive semidefinite matrix $\mathbf{L}^2$ (also save for a similarity transformation) [9]. It is worth to be noticed that such similarity transformations are not essential for an eigenproblem like (11) since the similarity matrices can be collected into a $\tilde{N} \times \tilde{N}$ diagonal matrix $\mathbf{S}$ to write (11) in the form

$$\mathbf{H}^H \mathbf{g}_s = E_s \mathbf{g}_s, \qquad s = 1, 2, \ldots, \tilde{N}, \tag{15}$$

with $\mathbf{H}^H$ Hermitian and $\mathbf{g}_s = \mathbf{S}^{-1}\mathbf{f}_s$.

Summarizing, we have found a nonrectangular grid on which $\mathbf{H}$ becomes a Hermitian matrix. Explicitly, if we choose the nodes $(r_i, \theta_j, \varphi_k)$ in such a form that the set r_i, $i = 1, \ldots, N$, satisfies (14), the set θ_j, $j = 1, \ldots, K$, satisfies (4), and $\varphi_k = -\pi + 2\pi k/M$, $k = 1, \ldots, M$, the projection of the Schrödinger equation on S becomes Eq. (11), where $\mathbf{H}$ is a Hermitian matrix given by (12). The spectrum of this matrix contains necessarily the exact binding energies of only one multiplet of the hydrogen atom, to, say the nth, provided $n \le N$ $(N \ge 2)$, $M \ge K \ge 2N - 1$, and $\varepsilon = 1/(2n^2)$. Since the matrices representing the partial differential operators constructed with these nodes yield exact values for polynomials of the form

$$\rho(r) P_l^m(\theta)_e^{im\varphi},$$

where $\rho(r)$ is a polynomial of degree at most $N-1$, $l = 0, 1, \ldots, (K-1)/2$, and $m = -l, \ldots, l$, the eigenfunctions of the multiplet divided by $e^{-\sqrt{2\varepsilon}r}$ [cf. (8)–(9)] are also determined exactly at the nodes save for a constant factor.

To do a numerical calculation it is necessary to choose first an index n, defining thus a multiplet and the parameter ε, and then the number of radial and angular nodes N, K, and M according to the relations already given. In addition to the exact eigenvalues of the nth multiplet, one can find in the spectrum of (11) eigenvalues approximating the energy of other multiplets defined by different indexes $n' \neq n$, $n' \leq N$. As expected, these eigenvalues converge numerically to their exact values of the first $(K-1)/2$ multiplets ($M \geq K \geq 2N-1$) as N grows.

It is noticing the existence of zero and positive eigenvalues in the spectrum of (11). In fact, the number of nonnegative eigenvalues is greater than the number of negative ones, but the numerical study of such eigenvalues is beyond the scope of this paper.

We show now some numerical results obtained through the diagonalization of (11) by standard double precision MATLAB functions using a personal computer. In Table I the negative eigenvalues of (11) with $N=4$ and $K=M=7$ are shown for $n=1, 2, 3, 4$ (in the last two cases only a part of them are displayed). In each column we find exact and approximated values for the binding energies of the hydrogen atom; the exact ones are those

TABLE I

Negative Eigenvalues of Eq. (11) with H Given by (12) for $N = 4$, $K = M = 7$, and $\varepsilon_n = 1/(2n^2)$ with $n = 1, \ldots, N$

ε_1	ε_2	ε_3	ε_4
1.00000000000000	1.00215707302795	1.03168585750231	1.08896461090157
2.04388882694316	1.99999999999993	2.00129478110128	2.00555350797036
2.04388882694346	2.00000000000000	2.00129478110130	2.00555350797038
2.04388882694354	2.00000000000000	2.00129478110132	2.00555350797038
2.09804764737169	2.00000000000000	2.00543455491769	2.06096113941247
	3.03156106874861	2.99999999999982	3.00051376536271
	3.03156106874867	2.99999999999990	3.00051376536275
	3.03156106874879	2.99999999999995	3.00051376536277
	3.03156106874883	2.99999999999999	3.00051376536278
	3.03156106874884	2.99999999999999	3.00051376536279
	3.09880783441467	2.99999999999999	3.01040973704290
	3.09880783441493	3.00000000000001	3.01040973704298
	3.09880783441499	3.00000000000002	3.01040973704302
	3.16392960609153	3.00000000000014	3.03184205479519
	5.34059520750606	4.06329322772771	3.99999999999962
	5.34059520750857	4.06329322772843	3.99999999999991
	5.34059520750915	4.06329322772855	3.99999999999995
	5.34059520750938	4.06329322772857	3.99999999999997
	5.34059520750947	4.06329322772861	3.99999999999997
	5.34059520750989	4.06329322772862	3.99999999999998
	5.34059520751064	4.06329322772872	4.00000000000000
		4.25955351771777	4.00000000000000
		4.25955351771817	4.00000000000001
		4.25955351771843	4.00000000000001
		4.25955351771845	4.00000000000001
		4.25955351771845	4.00000000000002
		4.70250143548207	4.00000000000004
		4.70250143548227	4.00000000000005
		4.70250143548250	4.00000000000033
			4.00000000000039

Note. The two rightmost columns show only some of the eigenvalues. In each case, the spectrum of (11) contains only one exact eigenvalue (counting the degeneracy) of the hydrogen atom. In order to distinguish this exact energy (corresponding to the nth multiplet), the value $1/\sqrt{-2E_s}$ is displayed.

TABLE II

Convergence of Some Negative Eigenvalues of Eq. (11) with H Given by (12) for $K = M = 7$ and $\varepsilon = 1/2$ to the Exact Energies of the First Three Multiplets of the Hydrogen Atom (Displayed as $1/\sqrt{-2E_j} = j,\ j = 1, 2, 3$) as N Grows

j	$N = 5$	$N = 10$	$N = 15$	$N = 20$
1	0.99999999999996	1.00000000000005	1.00000000000003	1.00000000000003
2	2.01049276733108	2.00000276409036	2.00000000023245	1.99999999999987
	2.01049276733135	2.00000276409060	2.00000000023589	2.00000000000002
	2.01049276733172	2.00000276409188	2.00000000023606	2.00000000000011
	2.02305632906585	2.00000703530320	2.00000000063539	2.00000000000116
3		3.01884262920929	3.00022234719467	3.00000127729828
		3.01884262920934	3.00022234720154	3.00000127729917
		3.01884262920941	3.00022234720269	3.00000127729919
		3.01884262921074	3.00022234720273	3.00000127730065
		3.01884262921528	3.00022234720280	3.00000127730920
		3.05122930639900	3.00072902585704	3.00000472833179
		3.05122930639920	3.00072902585744	3.00000472833209
		3.05122930640030	3.00072902585783	3.00000472833728
		3.07657778934264	3.00117867702690	3.00000812988290

Note. Each column contains again one exact eigenvalue. Since $\varepsilon = 1/2$, the exact energy corresponds to the first value in each column.

corresponding to the multiplet defined by the index n. In Table II we show the convergence of the approximated eigenvalues to their exact values when N grows, maintaining n, K, and M fixed ($n = 1$, $K = M = 7$). Since $n = 1$ ($\varepsilon = 1/2$), the first value of each column corresponds to the exact eigenvalue of the first multiplet. The choice for K and M yields convergence only for two other multiplets.

3. THE FINE STRUCTURE SPLITTING

We consider in this section the problem of a classical electron in a Coulomb field with the inclusion of spin effects in order to show some additional facts of the finite-dimensional representation of the angular momentum. We will apply our projection method to the Hamiltonian of this problem as it is given in the frame of perturbation theory and compare the eigenvalues of the discretized problem with the fine structure of the hydrogen atom.

3.1. *Total Angular Momentum*

We begin by giving the finite-dimensional representation of the total angular moment $\vec{J} = \vec{L} + \vec{S}$, which, according to the introduced method, is the $2\tilde{N} \times 2\tilde{N}$ vector matrix

$$\vec{\mathbf{J}} = 1_2 \otimes \vec{\mathbf{L}} + \vec{S} \otimes 1_{\tilde{N}}, \tag{16}$$

where $\tilde{N} = MK$, $\vec{\mathbf{L}}$ is the $\tilde{N} \times \tilde{N}$ vector matrix representing the angular momentum whose square is given by (2), and $\vec{S} = \vec{\sigma}/2$ is the intrinsic angular momentum of the electron, given, as is well-known, in terms of the Pauli matrices σ_x, σ_y, and σ_z. By using the expressions for L_x, L_y and L_z in terms of θ and φ and their derivatives, the components of $\vec{\mathbf{L}}$ can be

TABLE III
Eigenvalues λ_j of (18) Following the Sequence $\lambda_j = j(j+1)$, $1/2 \leq j \leq (K-1)/2$, for $K = M = 3, 5, 7$

$K = 3$	$K = 5$	$K = 7$
0.50000000000000 (4)	0.50000000000000 (4)	0.50000000000000 (4)
	1.50000000000000 (6)	1.50000000000000 (8)
	1.50000000000002	
	1.50000000000011	
		2.49999999999997
		2.49999999999999 (2)
		2.50000000000000 (8)
		2.50000000000001

Note. To distinguish them easily, the index $j = (-1 + \sqrt{1 + 4\lambda_j})/2$ is displayed. The digit between parentheses indicates the number of equal repeated eigenvalues.

written as[2]

$$\begin{aligned}
\mathbf{L}_x &= i(\sin\Phi \otimes D_\theta + \cos\Phi D_\varphi \otimes \cot\Theta),\\
\mathbf{L}_y &= -i(\cos\Phi \otimes D_\theta - \sin\Phi D_\varphi \otimes \cot\Theta),\\
\mathbf{L}_z &= -i D_\varphi \otimes 1_K.
\end{aligned} \tag{17}$$

Here, Φ is the diagonal matrix with entries $(\Phi)_{jk} = \varphi_j \delta_{jk}$. These components and their commutators can also be given in Cartesian coordinates, as is shown in the Appendix. Thus, $\mathbf{J}^2$ takes the form

$$\mathbf{J}^2 = \mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2, \tag{18}$$

where

$$\mathbf{J}_x = 1_2 \otimes \mathbf{L}_x + S_x \otimes 1_{\tilde{N}}, \qquad \mathbf{J}_y = 1_2 \otimes \mathbf{L}_y + S_y \otimes 1_{\tilde{N}}, \qquad \mathbf{J}_z = 1_2 \otimes \mathbf{L}_z + S_z \otimes 1_{\tilde{N}}.$$

The spectrum of (18) contains eigenvalues agreeing up to 15 digits with the exact values $j(j+1)$, $j = 1/2, 3/2, \ldots, l_{\max} - 1/2$, $l_{\max} = (K-1)/2$, $M \geq K$ (M and K odd numbers and $\hbar = 1$), as is shown in Table III for small values of $K = M$. Note that the total number of states is given correctly. The eigenvalues that do not follow the sequence $j(j+1)$ and the correct count disappear as the value of $K = M$ is increased. Thus, the projection scheme described at the beginning of this paper yields finite-dimensional representations of the quantum angular operators that also work quite well for spinor eigenproblems where the solution can be written in terms of products of trigonometric polynomials by certain functions powered to half-integer numbers (the eigenspinor functions of J_z and J^2). For other cases, the method requires one to take into account the behavior of the solution at the singularities of the differential equation or a further modification for nonseparable problems.

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[2] Actually, the sum of the squares of these expressions gives a matrix $(\mathbf{L}')^2$ different from $\mathbf{L}^2$, as is shown in the Appendix. Since the difference is essentially a projection matrix, the dimension of the linear space in which the use of $(\mathbf{L}')^2$ yields exact results becomes smaller than the one corresponding to the use of $\mathbf{L}^2$. This difference can be compensated by increasing M.

3.2. *The Perturbed Hamiltonian*

To compute the fine-structure splitting of the energy levels of the hydrogen atom we take the nonrelativistic reduction of the Hamiltonian

$$H_{op}^{nr} = H_{op}^{(0)} + \alpha^2\left[\frac{1}{2r^3}\vec{L}\cdot\vec{S} - \frac{1}{2}\left(H_{op}^{(0)} + 1/r\right)^2 + h_D\right] \tag{19}$$

obtained by perturbation theory. Here, the units used are those of the previous section, $\hbar$ has been withdrawn from $\vec{L}$ and $\vec{S}$, and $\alpha = e^2/(\hbar c)$ is the fine-structure constant. The unperturbed Hamiltonian $H_{op}^{(0)}$ is the one given in (7), and h_D is the Darwin interaction. The standard procedure computes the corrections to the energy levels by finding the matrix elements of the perturbed Hamiltonian (19) in the basis of the mutually commuting operators L^2, S^2, J^2, and J_z. We will find them instead through the projection of (19) in a polynomial space and the diagonalization of its finite-dimensional matrix representation obtained in this way.

The first point to address is the explicit form of the Darwin interaction to be projected. The singular and non-Hermitian term

$$h_D = -\frac{1}{4r^2}\frac{\partial}{\partial r} \tag{20}$$

is usually converted to the Hermitian form $-(1/8)\nabla^2(1/r) = (\pi/2)\delta(\vec{r})$ through an integration by parts. In order to give a finite-dimensional matrix representation of (19), we need to find, in particular, the discrete form of this Darwin term. Due to the difficulty of a numerical treatment of the delta function we find it more convenient to treat the non-Hermitian Darwin term (20) because it is easy to get the corresponding matrix form of (20), and numerical evidence shows that such a matrix has real eigenvalues when the radial nodes satisfies (14). Therefore, we will maintain (20) in (19) instead of the usual form $-(1/8)\nabla^2(1/r)$.

On the other hand, the addition of the spin–orbit interaction introduces an irregular singularity at $r = 0$, making it necessary to look for a change of variable that incorporates this behavior in the solution instead of (9). However, because of the smallness of α^2, we can keep the zeros of $L_N^{(1)}(2\sqrt{2\varepsilon}r)$ as the set of radial points even though this choice may give a lower convergence rate for the eigenvalues of (19) since it does not take properly into account the irregular singularity at the origin.

Thus, the change of variable (8) yields a new differential operator whose matrix form is

$$\mathbf{H}' = \mathbf{H}_0 + \frac{\alpha^2}{2}\left[\mathbf{r}^{-3}\vec{\mathbf{L}}\cdot\vec{S} - \left(\mathbf{H}_0 + \mathbf{r}^{-1}\right)^2 - \frac{1}{2}\mathbf{r}^{-2}(\mathbf{D}_r - \sqrt{2\varepsilon}\mathbf{1})\right], \tag{21}$$

where $\mathbf{H}_0 = 1_2 \otimes \mathbf{H}$, $\mathbf{H}$ given by (12), $\mathbf{r} = 1_{2NM} \otimes R$, $\mathbf{D}_r = 1_{2NM} \otimes D_r$, $\mathbf{1}$ is the identity matrix of dimension $2\tilde{N}$, and $\vec{L}\cdot\vec{S}$ is given by

$$2\vec{\mathbf{L}}\cdot\vec{S} = \sigma_x \otimes \mathbf{L}_x + \sigma_y \otimes \mathbf{L}_y + \sigma_z \otimes \mathbf{L}_z.$$

The last term of (21) is the form that the Darwin interaction takes after the change of variable (8). For numerical reasons and in order to identify the dependence of the eigenvalues on the quantum numbers n, l, and j, we find it more convenient to diagonalize the one-dimensional reduced version of (21)

$$H' = H_0 + \frac{\alpha^2}{2}\left[\lambda_{SL}R^{-3} - (H_0 + R^{-1})^2 - \frac{1}{2}R^{-2}(D_r - \sqrt{2\varepsilon}1_N)\right], \tag{22}$$

TABLE IV

Fine Structure of the Hydrogen Atom

(n, l, j)	$-E_{nlj}$	$-E_{nlj}^{50}$	$-E_{nlj}^{100}$	$-E_{nlj}^{800}$
$(1, 0, 1/2)$	0.50000665991795	0.50000613488955	0.50000639259060	0.50000662026219
$(2, 0, 1/2)$	0.12500208122436	0.12500195038954	0.12500201493321	0.12500207221205
$(2, 1, 1/2)$	0.12500208122436	0.12500208132882	0.12500208132927	0.12500208132965
$(2, 1, 3/2)$	0.12500041624487	0.12500041624486	0.12500041624487	0.12500041624488
$(3, 0, 1/2)$	0.05555629554644	0.05555623744838	0.05555626615153	0.05555629166215
$(3, 1, 1/2)$	0.05555629554644	0.05555629557858	0.05555629557882	0.05555629557903
$(3, 1, 3/2)$	0.05555580221918	0.05555580221948	0.05555580221949	0.05555580221949
$(3, 2, 3/2)$	0.05555580221918	0.05555580222221	0.05555580222221	0.05555580222221
$(3, 2, 5/2)$	0.05555563777676	0.05555563777706	0.05555563777706	0.05555563777706

Note. The exact binding energies $-E_{nlj}$ of the Hamiltonian (19) are compared with those obtained by the present method, $-E_{nlj}^{N}$, for $N = 50$, 100, 800.

where $H_0 = H_r + l(l+1)R^{-2}/2$, H_r is given by (13) and λ_{SL} take the value $l/2$ if $j = l + 1/2$ or $-(l+1)/2$ if $j = l - 1/2$, respectively. We display in Table IV the fine structure obtained by the diagonalization of (22) for the first three values of n. Again, we have used standard MATLAB functions and a personal computer to do the computations. Since the irregular singularity of the Hamiltonian has not been taken properly into account and the Darwin term leads to numerical difficulties, it is necessary to take large values of N, as shown in Table IV, to attain an agreement of the approximated eigenvalues $-E_{n0j}^{N}$ with the exact s-states within 8–9 digits (2–3 significant digits of the fine-structure correction to the Bohr energy levels), whereas for $l \neq 0$, the first 10–14 digits of the exact eigenvalues of the Hamiltonian (19) are attained for the first value of N (4–7 significant digits of the fine-structure correction), indicating that the matrix representation of the Darwin term, as expected, does not influence the states with $l \neq 0$. However, these eigenvalues do not show convergence to the exact energies as N grows. This is due to the fact that the factorization (8)–(9) does not take into account properly the behavior of the wave function at infinity even though it seems to work for $p_{3/2}$-states.

4. HYDROGEN ATOM IN A MAGNETIC FIELD

Let us consider the problem of a single electron bound by an atomic nucleus and a uniform magnetic field of intensity B pointing in the z-direction. By using the same units as before and $B_0 = m_e^2 e^3 c/\hbar^3 = 2.35 \times 10^9$ G as the unit of magnetic intensity such that $B = \beta B_0$ (β is the dimensionless magnetic field) and the gauge where $A_r = A_\theta = 0$, $A_\varphi = (Br \sin\theta)/2$ in spherical coordinates, the Schrödinger equation takes the form

$$\left[-\nabla^2 - i\beta\frac{\partial}{\partial\varphi} + \frac{1}{4}\beta^2 r^2 \sin^2\theta - \frac{2}{r} - \beta\right]\Psi = 2E\Psi, \tag{23}$$

where the spin of the electron is antialigned with the magnetic field in order to compute the ground state.

According to the present method we need to know the limit form $\Psi_\infty(r, \theta, \varphi)$ of Ψ for bound states [cf. (8)]. To this, we write $-E$ as ε and take the limit form of this equation as

$r \to \infty$ (assuming that the angular derivatives of the wave function are well-defined for all values of the angles) and obtain

$$\left[\frac{\partial^2}{\partial r^2} + i\beta\frac{\partial}{\partial\varphi} - \frac{1}{4}\beta^2 r^2 \sin^2\theta + \beta\right]\Psi_\infty = 2\varepsilon\Psi_\infty.$$

The φ-dependence of this equation can be factored to yield

$$\Psi_\infty(r,\theta,\varphi) = \Gamma(3/4 + a)U(a,x)e^{im\varphi}, \tag{24}$$

where

$$a = \frac{2\varepsilon - \beta(1-m)}{\beta\sin\theta}, \qquad x = \sqrt{\beta\sin\theta}\, r \tag{25}$$

are the arguments of the Weber parabolic function $U(a,x)$ (see [1]). The gamma function appearing in (24) is a normalization factor which makes Ψ_∞ independent of θ at $r = 0$.

Since our interest is to compute the ground energies, we take $m = 0$ and substitute $\Psi = \Psi_\infty f$ in (23) to yield

$$\left(f_{rr} + 2\frac{\gamma_r}{\gamma} f_r\right) + \frac{1}{r^2}\left(f_{\theta\theta} + 2\frac{\gamma_\theta}{\gamma} f_\theta\right) + \left[\frac{1}{r^2}\left(\frac{u_{\theta\theta}}{u} + \cot\theta\frac{u_\theta}{u}\right) + \frac{2}{r}\left(\frac{u_r}{u} + 1\right) + 2\varepsilon\right] f$$
$$+ \frac{1}{r^2\sin^2\theta} f_{\varphi\varphi} + i\beta f_\varphi = -2Ef, \tag{26}$$

where we have defined

$$\gamma(r,\theta) = r\sqrt{\sin\theta}\, u(r,\theta) \tag{27}$$

and $u(r,\theta) = \Gamma(3/4 + a)U(a,x)$, a and x given in (25) with $m = 0$.

We assume now that $f(r,\theta,\varphi)$ can be approximated by a function of the form $g(r,\theta)h(\varphi)$, where h is a (trigonometric) polynomial in φ and g is a polynomial in two variables (indeed, f has such a form for $\beta = 0$). This assumption allows us to project the part of (26) corresponding to the φ-coordinate according to the lines already discussed. Besides, since $g(r,\theta)$ yields N different trigonometric polynomials in θ when $r = r_j$, $j = 1, 2, \ldots, N$, and K different polynomials in r when $\theta = \theta_k$, $k = 1, 2, \ldots, K$, and the representation of the partial derivatives are given by blocks, we can demand that the kth block of the matrix representing $\partial/\partial r$ (in two variables) be constructed with the kth line of nodes r_j^k, $= 1, 2, \ldots, N$ according to the generic formula (5) and, similarly, that the jth (sparse) block of the matrix representing $\partial/\partial\theta$ be constructed with the line of nodes θ_k^j, $k = 1, 2, \ldots, K$ according to the generic formula (1). Let us denote these $KN \times KN$ matrices by $D_r^{(2)}$ and $D_\theta^{(2)}$, respectively. Therefore, the representation of $\partial/\partial r$, $\partial/\partial\theta$, and $\partial/\partial\varphi$ in (26) is given by

$$\mathbf{D}_r = 1_M \otimes D_r^{(2)}, \qquad \mathbf{D}_\theta = 1_M \otimes D_\theta^{(2)}, \qquad \mathbf{D}_\varphi = D_\varphi \otimes 1_{KN}. \tag{28}$$

The representation of a coefficient function in (26) becomes the tensor product of 1_M with the $KN \times KN$ diagonal matrix whose nonzero elements are the given function evaluated at the nodes (r_j^k, θ_k^j), $j = 1, 2, \ldots, N$, $k = 1, 2, \ldots, K$, with j running faster than k.

Thus, the discrete form of (26) is

$$\begin{aligned}&\left[\left(\mathbf{D}_r^2 + 2\mathbf{g}_\mathbf{r}\mathbf{D}_r\right) + \mathbf{r}^{-2}\left(\mathbf{D}_\theta^2 + 2\mathbf{g}_\theta\mathbf{D}_\theta\right) + \mathbf{r}^{-2}(\mathbf{u}_{\theta\theta} + \cot\boldsymbol{\Theta}\mathbf{u}_\theta) + 2\mathbf{r}^{-1}(\mathbf{u}_r + \mathbf{1}) + 2\varepsilon\mathbf{1}\right.\\ &\qquad \left. + \,\mathbf{c}\mathbf{D}_\varphi^2 + i\beta\mathbf{D}_\varphi\right]\mathbf{f} = -2E\mathbf{f}, \end{aligned} \tag{29}$$

where ε is taken as a trial parameter; E and $\mathbf{f}$ are expected to be approximants to the exact energy and eigenfunctions Ψ (the latter divided by Ψ_∞ and evaluated at the nodes); $\mathbf{D}_r$, $\mathbf{D}_\theta$, and $\mathbf{D}_\varphi$ are given in (28); $\mathbf{1}$ is the $MKN \times MKN$ identity matrix; and $\mathbf{g}_r$, $\mathbf{r}$, $\mathbf{g}_\theta$, $\mathbf{u}_{\theta\theta}$, $\cot\boldsymbol{\Theta}$, $\mathbf{u}_\theta$, $\mathbf{u}_\mathbf{r}$, and $\mathbf{c}$ are the diagonal matrices corresponding to the functions [cf. (27)] $\gamma_r/\gamma, r, \gamma_\theta/\gamma, u_{\theta\theta}/u$, $\cot\theta, u_\theta/u, \mathbf{u}_r/u$, and $1/(r^2\sin^2\theta)$, respectively. The nodes in the φ-coordinate can be chosen to be the equidistant points

$$\varphi_l = -\pi + \frac{2\pi l}{M}, \qquad l = 1, 2, \ldots, M, \tag{30}$$

in order to yield a similarity-transformed Hermitian matrix for $i\mathbf{D}_\varphi$ (see [9]), so that it remains to say how to choose the set of nodes (r_j^k, θ_k^j). To this end, we follow the ideas given in [2]. Let us denote by $\mathbf{d}_\mathbf{r}$ and $\mathbf{d}_\theta$ the diagonal entries of $\mathbf{D}_r$, and $\mathbf{D}_\theta$, respectively. If we impose the condition

$$\mathbf{d}_\mathbf{r} = -\mathbf{g}_\mathbf{r}, \qquad \mathbf{d}_\theta = -\mathbf{g}_\theta, \tag{31}$$

then $-\mathbf{D}_r^2 - 2\mathbf{g}_\mathbf{r}\mathbf{D}_r$ and $-\mathbf{D}_\theta^2 - 2\mathbf{g}_{\boldsymbol\theta}\mathbf{D}_{\boldsymbol\theta}$ are positive semidefinite matrices (save for a similarity transformation) and therefore, the eigenvalues of (29) are real. Written in detail, (31) becomes the system of $2KN$ nonlinear equations

$$\begin{aligned} \sum_{l=1}^{N}{}' \frac{1}{\left(r_j^k - r_l^k\right)} + \frac{\gamma_r\left(r_j^k, \theta_k^j\right)}{\gamma\left(r_j^k, \theta_k^j\right)} &= 0,\\ \sum_{l=1}^{K}{}' \frac{1}{2}\cot\frac{\left(\theta_k^j - \theta_l^j\right)}{2} + \frac{\gamma_\theta\left(r_j^k, \theta_k^j\right)}{\gamma\left(r_j^k, \theta_k^j\right)} &= 0, \end{aligned} \tag{32}$$

where $j = 1, 2, \ldots, N$, $k = 1, 2, \ldots, K$ and $\gamma(r, \theta)$ is given by (27). Thus, if β and ε are given, the set of nodes (r_j^k, θ_k^j) can be found by solving (32).

Therefore, once we have determined the equations for the nodes, we can proceed to solve the eigenproblem (29). To obtain an eigenvalue of (29) for a given value β' of parameter β, we follow a recursive procedure on the parameters β and ε consisting in the following steps. We begin with the nodes yielding exact results for $\beta = 0$ and $\varepsilon = 1/2$. These nodes are used as initial points to solve (32) with β equal to some small increment. The new nodes are used to construct and solve (29), obtaining a ground eigenvalue used as a value of ε in the next calculation. We increment again β and use the last set of nodes as initial points to find a new set of nodes through (32) with the actual values of β and ε. Solving again (29), we find a new ε, and so on. We stop the procedure when $\beta = \beta'$, yielding thus an eigenvalue for the ground state. Now we change the increment of β and the procedure is restarted. After several trials we search for the stabilized digits in the eigenvalues obtained in this way. In order to increase a bit the accuracy of results and admit even numbers K, one can use the

TABLE V

Binding Energies $-E_0(M, K, N)$ of the Ground State of a Hydrogen Atom in a Uniform Magnetic Field Computed According to the Present Method

β	$-E_0(3,4,4)$	$-E_0(3,6,6)$	$-E_0(3,8,8)$	$-E_0$
0.0001	0.500 049 997 500	0.500 049 997 500	0.500 049 997 500	0.500 049 997 500
0.001	0.500 499 750 00	0.500 499 750 000	0.500 499 750 000	0.500 499 750 000
0.01	0.504 961	0.504 975	0.504 975	0.504 975 002 759
0.1	0.547 518	0.547 527	0.547 525	0.547 526 480 401
0.4	0.664 7	0.664 7	0.664 6	0.664 605 379 868
0.6	0.727	0.727 7	0.727 3	0.727 462 287 757
0.8	0.78	0.782	0.782	0.782 283 393 769
1.0	0.83	0.83	0.83	0.831 168 896 733

Note. Only the first stable digits obtained through the recursive procedure described in Section 4 are shown. They are compared with the energies $-E_0$ given in [10].

matrix representation of $d/d\theta$,

$$D\theta = S\bar{D}S^{-1},$$

$$\bar{D}_{ij} = \begin{cases} \sum_{l=1}^{\prime K} \cot(\theta_i - \theta_l), \, i = j, \\ \cot(\theta_i - \theta_j), \, i \neq j, \end{cases} \qquad S_{ij} = \delta_{ij} \prod_{l \neq j}^{K} \sin(\theta_j - \theta_l),$$

given in [4]. In such a case, $D_\theta^{(2)}$ will change accordingly [so does (28)] and the summand of the second equation in (32) will change to $\cot(\theta_k^j - \theta_l^j)$. This is what we do to compute the ground energies shown in Table V for $N = 4, 6, 8$; $K = N$; and $M = 3$. These values are compared with those given in [10]; only the stable digits obtained through our recursive procedure (described above) are shown. As can be seen, the present method yields acceptable results only for small β. This is due to the fact that (24) becomes an oscillatory function when $a < 0$ [or $\beta > 2\varepsilon$; cf. Eq. (25)], producing that the solution of (32) cannot be found with high precision for $\beta \approx 1$. For $\beta \gg 1$, the solution of (32) is not unique, so another function Ψ_∞ should be chosen.

We end this section by noting that this problem can also be solved numerically in two variables (r and θ) if we just ignore the dependence of the wave function on the coordinate φ. However, we have preferred to show the results obtained by using three coordinates instead of only two in order to give a complete numerical treatment of this problem, even though numerical calculations in two variables yield the same results.

5. FINAL COMMENT

As we have shown, the method introduced in this paper can be easily implemented for eigenproblems whose solution can be expressed in terms of products of polynomials, yielding accurate eigenvalues and eigenfunctions (obtained from the eigenvectors through an interpolation) for small values of the number of nodes used to construct the matrix representations of the partial derivatives. However, this technique depends strongly on the correct choice of the boundary function that defines the nodes, and so the selection of this function becomes crucial in order to attain convergence to exact solutions of more complicated problems. The modification of the procedure introduced in the preceding section yields acceptable results only for mildly nonseparable problems.

APPENDIX

We show here the form that the algebra of the angular momentum takes in a finite-dimensional linear space and explain why the sum of the squares of (17) becomes different from (2). We will see that such a difference appears as an intrinsic characteristic of the projection of the angular operators on a finite-dimensional space.

We begin by computing the commutators $[D_\varphi, \sin\Phi]$ and $[D_\varphi, \cos\Phi]$. Using standard trigonometric relations, we get that

$$D_\varphi \sin\Phi = \sin\Phi D_\varphi + \cos\Phi - U_c \tag{33}$$

and

$$D_\varphi \cos\Phi = \cos\Phi D_\varphi - \sin\Phi + U_s, \tag{34}$$

where U_c and U_s are projection matrices defined by

$$(U_c)_{jk} = (-1)^{j+k} \cos\left(\frac{\varphi_j + \varphi_k}{2}\right), \qquad (U_s)_{jk} = (-1)^{j+k} \sin\left(\frac{\varphi_j + \varphi_k}{2}\right).$$

These matrices can be joined to form the complex matrix $U = U_c + iU_s$, which projects a trigonometric polynomial

$$f_m(\varphi) = \sum_{l=-m}^{m} c_l e^{il\varphi}, \qquad m \le m_{\max} = (M-1)/2,$$

on the components of higher degree $m_{\max}$. To make this clear, let us take the polynomials $\cos\varphi f_m(\varphi)$, $\sin\varphi f_m(\varphi)$, and calculate their derivatives by using D_φ. Since the use of D_φ yields exact results at the nodes for polynomials of degree at most $m_{\max}$, the formulae

$$D_\varphi \sin\Phi F_m = \sin\Phi D_\varphi F_m + \cos\Phi F_m \qquad D_\varphi \cos\Phi F_m = \cos\Phi D_\varphi F_m - \sin\Phi F_m$$

must hold whenever $m \le m_{\max} - 1$. Here, F_m is the vector of values of $f_m(\varphi_j)$. Therefore, comparing these expressions with (33) and (34), we see that our assertion about U follows.

We calculate now the sum $\mathbf{L}_x^2 + \mathbf{L}_y^2$. According to (17), we find that

$$\begin{aligned} -\left(\mathbf{L}_x^2 + \mathbf{L}_y^2\right) = \mathbf{D}_\theta^2 &+ (\cos\Phi D_\varphi \sin\Phi - \sin\Phi D_\varphi \cos\Phi) \otimes \cot\Theta D_\theta \\ &+ (\cos\Phi D_\varphi \cos\Phi + \sin\Phi D_\varphi \sin\Phi)\, D_\varphi \otimes \cot^2 \otimes. \end{aligned} \tag{35}$$

With $\mathbf{L}'^2 = \mathbf{L}_x^2 + \mathbf{L}_y^2 + \mathbf{L}_y^2$, the substitution of (33) and (34) in (35) gives

$$-\mathbf{L}'^2 = -\mathbf{L}^2 - U_c' \otimes \cot\Theta D_\theta + U_s' D_\varphi \otimes \cot^2\Theta,$$

where $\mathbf{L}^2$ is given by (2) and

$$U_c' = \cos\Phi U_c + \sin\Phi U_s, \qquad U_s' = \cos\Phi U_s - \sin\Phi U_c.$$

Since the components of these two matrices are given by

$$(U_c')_{jk} = (-1)^{j+k} \cos\left(\frac{\varphi_j - \varphi_k}{2}\right), \qquad (U_s')_{jk} = (-1)^{j+k+1} \sin\left(\frac{\varphi_j - \varphi_k}{2}\right),$$

and the nodes φ_j are symmetrically located in $[-\pi, \pi]$, U'_c and U'_s are the product of a permutation matrix by U_c and U_s, respectively. Therefore, $\mathbf{L}^2$ and $\mathbf{L}'^2$ both yield the same results when applied to vectors formed through tensor products of polynomials in θ and φ of degrees at most $(K-1)/2$ and $(M-3)/2$, respectively, evaluated at the nodes.

Now, we address the question of the form that the commutators of the components of the angular momentum take in a finite-dimensional space. Let us take N points on the axis x, M on y, and K on z, to form the set of Cartesian nodes (x_n, y_m, z_k), and the diagonal matrices representing the variables x, y, and z,

$$\begin{aligned} \mathbf{X} &= (1_K \otimes 1_M \otimes X), \\ \mathbf{Y} &= (1_K \otimes Y \otimes 1_N), \\ \mathbf{Z} &= (Z \otimes 1_M \otimes 1_N). \end{aligned}$$

The main diagonals of X, Y, and Z contain the sets of points x_n, y_m, and z_k, respectively. On account of (5), the $NMK \times NMK$ matrices

$$\begin{aligned} \mathbf{D}_x &= (1_K \otimes 1_M \otimes D_x), \\ \mathbf{D}_y &= (1_K \otimes D_y \otimes 1_N), \\ \mathbf{D}_z &= (D_z \otimes 1_M \otimes 1_N), \end{aligned}$$

are the representations of the partial derivatives $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$ in a polynomial subspace. Thus, the matrix components of the angular momentum in Cartesian coordinates (with $\hbar = 1$) become

$$\begin{aligned} \mathbf{L}_x &= -i(\mathbf{YD}_z - \mathbf{ZD}_y), \\ \mathbf{L}_y &= -i(\mathbf{ZD}_x - \mathbf{XD}_z), \\ \mathbf{L}_z &= -i(\mathbf{XD}_y - \mathbf{YD}_x). \end{aligned} \tag{36}$$

By using (5), it is easy to see that the commutators of (36) are given by

$$\begin{aligned} [\mathbf{L}_x, \mathbf{L}_y] &= i\mathbf{L}_z - U_z \otimes (D_y \otimes X - Y \otimes D_x), \\ [\mathbf{L}_y, \mathbf{L}_z] &= i\mathbf{L}_x - (D_z \otimes Y - Z \otimes D_y) \otimes U_x, \\ [\mathbf{L}_z, \mathbf{L}_x] &= i\mathbf{L}_y - (Z \otimes U_y \otimes D_x - D_z \otimes U_y \otimes X), \end{aligned} \tag{37}$$

where $U_\alpha = P_\alpha O_\alpha P_\alpha^{-1}$ (the index α stands for x, y, or z), O_α is a matrix of dimension equal to the number of nodes in use and elements all equal to 1, and P_α has the structure given in (5). O_α is again a projection matrix and so is U_α. To see this, let us consider a polynomial $f(x)$ of degree at most $N-2$ and construct a vector F by evaluating $f(x)$ at the x-nodes. Since the coefficient of x^{N-1} of the Lagrange representation of $f(x)$ must vanish, any $f(x)$ satisfies

$$\sum_{l=1}^{N} \frac{f(x_l)}{p'(x_l)} = 0,$$

$p(x) = \prod_{l=1}^{N}(x - x_l)$ [cf. (5)], yielding

$$\left(O_x P_x^{-1} F\right)_j = 0,\ j = 1, 2, \ldots, N.$$

Thus, U_x projects a vector on the component corresponding to x_α^{N-1} and therefore, (37) gives the expected result if we multiply them by any vector of the subspace of tensor polynomials of degree at most $N-2$ in x, $M-2$ in y, and $K-2$ in z.

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