

# Pseudospectral methods for atoms in strong magnetic fields

Jeremy S. Heyl<sup>†</sup> and Anand Thirumalai

*Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Z1*

<sup>†</sup> *Email: heyjl@phas.ubc.ca; Canada Research Chair*

Accepted 2010 April 27. Received 2010 April 23; in original form 2010 April 2

## ABSTRACT

We present a new pseudospectral algorithm for the calculation of the structure of atoms in strong magnetic fields. We have verified this technique for one, two and three-electron atoms in zero magnetic fields against laboratory results and find typically better than one-percent accuracy. We further verify this technique against the state-of-the-art calculations of hydrogen, helium and lithium in strong magnetic fields (up to about  $2 \times 10^6$  T) and find a similar level of agreement. The key enabling advantages of the algorithm are its simplicity (about 130 lines of commented code) and its speed (about  $10^2 - 10^5$  times faster than finite-element methods to achieve similar accuracy).

**Key words:** physical data and processes: atomic data — physical data and processes: magnetic fields — stars: neutron — stars: magnetic fields — stars: white dwarfs

## 1 INTRODUCTION

A hydrogen atom in a magnetic field is arguably the simplest Hamiltonian without an analytic solution – it is a combination of a harmonic oscillator with a Coulomb potential. The problem of atoms in magnetic fields is also a vexing challenge in the study of neutron stars and white dwarfs. A sufficiently intense magnetic field cannot be treated perturbatively. If the magnetic field completely dominates over the nucleus one can understand the atomic structure as a one-dimensional atom (Loudon 1959; Haines & Roberts 1969). A non-trivial relaxation of the one-dimensional assumption is the adiabatic approximation that assumes that the wavefunction of the electron perpendicular to the magnetic field is simply the ground Landau level of the electron without the nucleus (e.g. Heyl & Hernquist 1998).

The most challenging regime is of course where the nucleus and the magnetic field compete for the electron’s attention. This lies around  $10^{4-6}$  T for hydrogen and is known as the strong-field regime. For such field strengths one cannot assume that the electron lies in the lowest Landau level. For a detailed bibliography of the vast literature of atomic calculations in strong magnetic fields, we encourage the reader to consult our recent work (Thirumalai & Heyl 2009).

In the strong-field regime, one can assume that the wavefunction is a sum of Landau levels or spherical harmonics (e.g. Ruder et al. 1994) or solve the two-dimensional partial differential equation without this assumption (e.g. Thirumalai & Heyl 2009). This work takes the second approach and solves the differential equations for the electronic wavefunctions and the interelectron potentials numerically.

The main goal of this paper is not to present more accurate calculations of atoms in strong magnetic fields (although the calculations rival the current state of the art), but rather the purpose is to provide a new, much faster algorithm to perform these calculations and verify its results against previous work.

This new algorithm is straightforward to implement and compact; the thirty-line program for single-electron atoms and the 130-line program for multiple-electron atoms are presented in the appendices. With this simplicity comes a dramatic speed-up of the calculation of a factor of  $10^2 - 10^5$  relative to finite-element techniques (Thirumalai & Heyl 2009) while achieving similar accuracy. This pseudospectral algorithm interpolates the approximate solution to the differential equations as a polynomial over an irregular mesh. Because the approximate solution is a polynomial, it is also analytic over the mesh. Even if the actual solution oscillates on a scale of a couple of mesh points, the analytic interpolant still provides an accurate approximation to the solution. On the other hand, if the actual solution develops discontinuities (i.e. it is not analytic), the pseudospectral method is less useful, (however see Boyd 2001). In the case of magnetized atoms, the solution to the Schrodinger equation is analytic everywhere except at the origin where we can set a boundary condition, so the pseudospectral method yields great returns.

In the next sections we will present the partial differential equations for the electronic wavefunctions (§2.1), the interelectron potential (§2.2), an introduction to pseudospectral methods (§2.3), the application of boundary conditions (§2.4), our results (§3) and source code (Appendices A-B).

## 2 CALCULATIONS

### 2.1 The Hamiltonian

Rather than examine the Hamiltonian of an atom in a magnetic field in detail, we will simply recap the relevant equations here and refer the reader to Thirumalai & Heyl (2009) for further details. We use the Hartree-Fock equations to describe the wavefunction of a multiple-equation system, this yields a coupled set of Schrodinger-like equations for an approximation to the wavefunction of each electron,

$$\left[ -\nabla^2 - \frac{2}{r_s} + \beta_Z^2 R_\perp^2 + \frac{2}{Z} \sum_{j,j \neq i} V_{ij} - E_j \right] \psi_i = 0 \quad (1)$$

where  $i, j = 1, 2, 3, \dots, N$ . Here  $N$  is the number of electrons,  $Z$  is the charge of the nucleus located at the origin,  $V_{ij}$  is the inter-electron potential operator and  $\beta_Z$  measures the strength of the magnetic field,  $\beta_Z = Be\hbar/(2Z^2\alpha^2 m_e^2 c^2) = B/(4.7Z^2 \times 10^5 \text{T})$ . The variable  $r_s$  is the distance from the origin and  $R_\perp = r_s \sin \theta$ , the distance from the axis defined by the direction of the magnetic field; this notation is consistent with the software in the appendices. The functions  $\psi_i$  must be finite at the origin and approach zero as  $\mathbf{r} \rightarrow \infty$ .

The total binding energy of the atom is given by

$$E = \sum_i \left[ E_i + 2\beta_Z \left( m_i + s_i - \frac{1}{2} \right) - \frac{1}{Z} \sum_{j,j \neq i} \langle \psi_i | V_{ij} | \psi_i \rangle \right] \quad (2)$$

in units of  $Z^2 \alpha^2 m_e c^2 / 2$

Although the Hamiltonian is no longer spherically symmetric, it is still symmetric about the magnetic axis, so we expect the azimuthal or magnetic quantum number  $m_i$  to be good. We will label the solutions to Eq. (1) by  $\nu_i, s_i$  and  $m_i$  where  $s_i$  is the spin of the electron and  $\nu_i$  equals 1 for the most bound state with a particular value of  $s_i$  and  $m_i$  and 2 for the next most bound state and so on.

The first step is to specify the precise differential equations to solve. Specifically, we will take

$$\psi_i = \frac{u_i(r, \mu)}{r_s} e^{im_i \phi} \quad (3)$$

The parameter  $\mu = \cos \theta$ , where  $\theta$  is the angle from the z-axis. For the radial dependence, the domain is  $[0, \infty)$ , so we would like compactify the domain to  $[-1, 1]$ . Let

$$r = 2 \tanh \frac{r_s}{r_Z} - 1 \quad (4)$$

where  $r_s$  ranges from zero to infinity while  $r$  now ranges from  $-1$  to  $1$ . The quantity  $r_Z$  is the ‘‘zoom radius’’ that determines at what value of  $r_s$  the relationship between  $r$  and  $r_s$  goes from linear to exponential,

$$r \approx 2 \frac{r_s}{r_Z} - 1, r \ll r_Z; r \approx 1 - 4 \exp(-2r_s/r_Z), r \gg r_Z. \quad (5)$$

Because  $2 \tanh 1 - 1 \approx 0.5$  about one third of the points lie at  $r > r_Z$ . Because the domain is compactified we can easily apply boundary conditions both at infinity and at the origin as appropriate for solving the Schrodinger equation:  $u_i(-1, \mu) = u_i(+1, \mu) = 0$  and the additional condition for  $m_i \neq 0$  that  $u_i(r, -1) = u_i(r, +1) = 0$ .

Using the substitution of Eq. (3) into (1), yields

$$\left[ -\frac{\partial^2}{\partial r_s^2} - \frac{1}{r_s^2} (1 - \mu^2) \frac{\partial^2}{\partial \mu^2} + \frac{2\mu}{r_s^2} \frac{\partial}{\partial \mu} + \frac{m_i^2}{R_\perp^2} - \frac{2}{r_s} \right.$$

$$\left. + \beta_Z^2 R_\perp^2 + \frac{2}{Z} r_s e^{-im_i \phi} \sum_{j,j \neq i} V_{ij} \frac{e^{im_i \phi}}{r_s} - E_j \right] u_i = 0 \quad (6)$$

where

$$\frac{\partial^2}{\partial r_s^2} = 4 (1 - r_p^2) \left[ (1 - r_p^2) \frac{\partial^2}{\partial r^2} - r_p \frac{\partial}{\partial r} \right] \quad (7)$$

where  $r_p = (r + 1)/2$ .

### 2.2 Inter-electron potential

Using the results of §2.3 we can convert this partial differential equation into a matrix equation, specifically an eigenvalue equation. However, before doing this in §2.4, we must discuss the inter-electron potential  $V_{ij}$ .

The inter-electron potential consists of two terms, the direct and exchange interactions where

$$V_{ij} = V_{\text{direct},ij} - V_{\text{exchange},ij} \quad (8)$$

if the spins of electrons  $i$  and  $j$  are aligned and  $V_{ij} = V_{\text{direct},ij}$  otherwise. The direct interaction satisfies

$$V_{\text{direct},ij} \psi_i = \phi_j(\mathbf{r}) \psi_i \quad (9)$$

where

$$\nabla^2 \phi_j = -4\pi \psi_j^* \psi_j \quad (10)$$

which we can solve, knowing the values of  $\psi_j$ , by inverting the Laplacian to yield

$$\phi_j = (\nabla^2)^{-1} [-4\pi \psi_j^* \psi_j] \quad (11)$$

where  $(\nabla^2)^{-1}$  is the inverse of the Laplacian with the appropriate boundary conditions supplied. Therefore, the direct interaction is a diagonal operator, essentially a function.

On the other hand the exchange interaction is more complicated. We have

$$V_{\text{exchange},ij} \psi_i = \tilde{\phi}_{ij}(\mathbf{r}) \psi_j \quad (12)$$

where

$$\nabla^2 \tilde{\phi}_{ij} = -4\pi \psi_j^* \psi_i. \quad (13)$$

Therefore, we have

$$V_{\text{exchange},ij} \psi_i = \tilde{\phi}_{ij}(\mathbf{r}) \psi_j = \psi_j (\nabla^2)^{-1} [-4\pi \psi_j^* \psi_i]. \quad (14)$$

Thinking of the different components of the right-hand sides of Eqs. (12) and (15) as matrices, we can write the potentials due to the direct and exchange interactions in matrix notation as

$$V_{\text{exchange},j} = -4\pi \text{diag}(\psi_j) (\nabla^2)^{-1} \text{diag}(\psi_j^*) \quad (15)$$

where we have dropped the index  $i$  because the exchange interaction operator only depends on the wavefunction of the electron  $j$ . Both the direct and exchange potentials must go to zero at  $\mathbf{r} \rightarrow \infty$  and be finite at the origin.

The set of coupled equations is of course non-linear and difficult to solve directly; however, we can approach the solution iteratively, by first solving the equations (1) ignoring the inter-electron terms and then on subsequent iterations using the wavefunctions from the previous iteration to calculate the interaction operator using Eq. (11) and (15). At each iteration the equations are decoupled, so the time to

calculate a single iteration scales as the number of electrons, making the calculation of even large atoms tractable. If the equations were coupled through the exchange term, then each dimension of the matrix to diagonalize would scale with the number of electrons so the time to complete an iteration would scale as the cube of the number of electrons.

Let's evaluate for the exchange potential operator using the substitution of Eq. (3). We have

$$V_{\text{exchange},ij} \left( u_i \frac{e^{im_i\phi}}{r_s} \right) = \tilde{\phi}_{ij}(\mathbf{r}) u_j \frac{e^{im_j\phi}}{r_s} \quad (16)$$

and

$$r_s e^{-im_i\phi} V_{\text{exchange},ij} \left( \frac{e^{im_i\phi}}{r_s} u_i \right) = \tilde{\phi}_{ij}(\mathbf{r}) u_j e^{-im_j\phi} \quad (17)$$

where  $\Delta m = m_i - m_j$ . Because none of the other terms in the Hamiltonian depend of  $\phi$ , neither side of Eq. (17) can depend on  $\phi$  so let us define

$$\tilde{\phi}_{ij}(\mathbf{r}) = \tilde{\phi}_{ij}^{\Delta m}(r_s, \mu) e^{i\Delta m\phi} \quad (18)$$

where

$$\nabla^2 \left( \tilde{\phi}_{ij}^{\Delta m}(r_s, \mu) e^{i\Delta m\phi} \right) = -4\pi \frac{u_j^* u_i}{r_s^2} e^{i\Delta m\phi}. \quad (19)$$

Simplifying this result yields

$$\left( \nabla^2 - \frac{\Delta m^2}{R_{\perp}^2} \right) \tilde{\phi}_{ij}^{\Delta m}(r_s, \mu) = -4\pi \frac{u_j^* u_i}{r_s^2} \quad (20)$$

and

$$\begin{aligned} r_s e^{-im_i\phi} V_{\text{exchange},ij} \frac{e^{im_i\phi}}{r_s} \\ = -4\pi \text{diag}(u_j) \left( \nabla^2 - \frac{\Delta m^2}{R_{\perp}^2} \right)^{-1} \text{diag} \left( \frac{u_j}{r_s^2} \right) \end{aligned} \quad (21)$$

where

$$\nabla^2 = \frac{\partial^2}{\partial r_s^2} + \frac{1}{r_s^2} (1 - \mu^2) \frac{\partial^2}{\partial \mu^2} - \frac{2\mu}{r_s^2} \frac{\partial}{\partial \mu}. \quad (22)$$

The result for the direct interaction is nearly trivial because it is a function rather than an operator. We have

$$r_s e^{-im_i\phi} V_{\text{direct},ij} \left( \frac{e^{im_i\phi}}{r_s} u_i \right) = -4\pi (\nabla^2)^{-1} \left[ \frac{u_j^2}{r_s^2} \right] \quad (23)$$

We must specify the boundary conditions on the inverse operators in Eq. (21) and (23). Both the direct and exchange potentials must go to zero at  $\mathbf{r} \rightarrow \infty$  and be finite at the origin. Furthermore, for  $\Delta m \neq 0$ , the exchange potential must vanish along the magnetic axis.

In principle one could solve for all of the electronic wavefunctions at the same time, but this would render the differential equations non-linear; therefore, we first neglect the electronic contribution to the potential to find a first guess at the electronic wavefunctions. These wavefunctions become the input into Eq. (21) and (23) for the second iteration. This process is repeated until the total energy of the state is constant to one part in  $10^5$  between successive iterations.

### 2.3 Pseudospectral methods

The basic idea behind interpolating spectral (or pseudospectral) methods is to approximate functions by their values at

a set of points and a set of smooth functions to interpolate between these points for the purpose of calculating derivatives and integrals. An example is useful to make this concrete. A function  $f(x)$  takes the values  $f_i$  at the points  $x_i$ . We could construct an interpolation scheme by linearly interpolating between the points or using a cubic spline. This is the basis of finite difference schemes with successively higher accuracy. However, if we wanted an analytic function through the points we could use the polynomial that passes through all of the points. This polynomial interpolant is given by

$$f_I(x) = \sum_i f_i p_i(x) = \sum_i f_i \frac{\prod_{j \neq i} (x - x_j)}{\prod_{j \neq i} (x_i - x_j)} \quad (24)$$

where we have used the notation of Trefethen (2000). The polynomial  $p_i(x)$  has the property that it takes the value of unity at  $x_i$  and it vanishes at all of the other points where the function values are given. We can take the derivative of the basic polynomial to yield

$$p_i'(x) = p_i(x) \sum_{j \neq i} (x - x_j)^{-1} \quad (25)$$

and evaluate it at one of the points  $x_k$  to yield

$$p_i'(x_k) = p_i(x_k) \sum_{j \neq i} (x_k - x_j)^{-1} = D_{ik} \quad (26)$$

where

$$D_{ik} = \frac{\prod_{j \neq i, k} (x_k - x_j)}{\prod_{j \neq i} (x_i - x_j)}, D_{ii} = \sum_{j \neq i} (x_i - x_j)^{-1} \quad (27)$$

where  $D_{ik}$  is the differentiation matrix such that  $f_I'(x_k) = D_{ik} f_i$ . Unlike finite element, finite volume and finite difference techniques, the differentiation matrix is dense, so it is more costly to manipulate; however, one can often achieve similar accuracy with much smaller matrices for problems with smooth solutions. This decrease in the size of the matrices more than offsets the burden of handling dense matrices.

The choice of the points  $x_i$  is completely arbitrary but for finite domains it is more stable to pick the points to be bunched toward the ends of the domain and more sparse in the middle (Trefethen 2000). A convenient set of points over the domain  $[-1, 1]$  are the Chebyshev points

$$x_i = \cos(i\pi/N), i = 0 \dots N. \quad (28)$$

This domain is well suited for the angular dependence in spherical coordinates where we define  $\mu = \cos \theta = z/r$  and use the Chebyshev points to sample  $\mu$ . Thus the angular dependence is evenly sampled in  $\theta$ .

### 2.4 Discrete equations

The `Octave` programs given in the appendices for the single and multiple-electron problems convert the partial differential equations of §2.1 and 2.2 to matrix equations using the pseudospectral methods outlined in §2.3. We encourage readers that are familiar with `Octave` or `Matlab` to look under the hood and dissect the routines.

The previous section outlined how to construct a differentiation matrix using a pseudospectral method in one dimension. The second derivative is simply the square of this

matrix and an integration operator is the inverse of the differentiation matrix with some boundary condition supplied. The remaining subtleties are how to apply boundary conditions and how to move to more than one dimension. The techniques outlined here are presented in Trefethen (2000) in greater detail, clarity and generality.

Supplying the boundary conditions for the eigenvalue equations is rather straightforward and most easily illustrated by an example. Let us find the eigenvalues of the matrix  $M$  with the solution  $f$  vanishing at the end points. We have

$$Mf = \lambda f. \quad (29)$$

Let's define the diagonal matrix,

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & & & \ddots & & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix} \quad (30)$$

with all of the diagonal elements unity except for the first and last that vanish. Multiplying the vector  $\vec{f}$  by  $B$  has the effect of setting the endpoints to zero, so let's look at the following eigenvalue equation

$$BMB\vec{f} = \lambda\vec{f}. \quad (31)$$

The matrix  $B$  that precedes  $M$  ensures that the resulting output vector satisfies the boundary conditions, and the matrix that follows  $M$  ensures that the input vector satisfies the boundary conditions as well, so the eigenvectors of the matrix  $BMB$  except for two are guaranteed to satisfy the boundary conditions. The two remaining eigenvectors are linear combinations of  $[1\ 0 \cdots 0\ 0]$  and  $[0\ 0 \cdots 0\ 0\ 1]$  and have zero eigenvalues. We can either ignore these eigenvectors or define a new matrix  $\tilde{M}$  that lacks the first and last columns and the first and last rows of the original matrix  $M$ . The eigenvectors of  $\tilde{M}$  are the same as those of  $BMB$  but with the first and last entries omitted.

In summary, to obtain the set of eigenvectors of  $M$  that satisfy the boundary conditions we construct  $\tilde{M}$  and add the first and last entries if needed. For the potential calculation it is often more useful to work with  $BMB + (I - B)$  so that the resulting matrix can be inverted before setting the boundary conditions. In the potential calculation we set the boundary condition at infinity because the Laplacian matrix vanishes for the row and column corresponding to infinity, so we drop the row and column before inverting the Laplacian. However, we would also like to set a boundary condition at the origin, so we must include the origin in the calculation. At the origin the angular terms in the Laplacian diverge, but this is a coordinate singularity that we address by including only a single entry for the origin and drop the angular derivatives there. In this way, we address the divergent terms at the origin and the vanishing terms at infinity.

The second issue is how to build the various operators in more than one dimension. Let's say that we have obtained a vector of points  $\vec{x}$  of dimension  $N$  and a pseudospectral derivative  $D_x$  and similarly a vector of points  $\vec{y}$  of dimension  $M$  and its derivative  $D_y$ . If we construct

$$\vec{x}' = \vec{x} \otimes \vec{1}_M, \vec{y}' = \vec{1}_N \otimes \vec{y} \quad (32)$$

where  $\vec{1}_N$  is a vector of  $N$  ones and  $\otimes$  denotes the Kronecker product, we obtain a two-dimensional mesh  $(\vec{x}', \vec{y}')$  of points in two vectors of dimension  $N \times M$ . Finally we would like to construct the Laplacian over this mesh (this example is Cartesian). We have

$$\nabla^2 = (D_x)^2 \otimes I_M + I_N \otimes (D_y)^2. \quad (33)$$

where  $I_N$  is the  $N \times N$ -identity matrix. The resulting matrix  $\nabla^2$  has dimensions  $(N \times M) \times (N \times M)$  and calculates the Laplacian over the mesh specified by  $(\vec{x}', \vec{y}')$ .

These techniques allow us to discretize the equations outlined in §2.1 and 2.2 to obtain the software in the appendices.

## 3 RESULTS

### 3.1 Hydrogen

As a first test of the algorithm, we examined hydrogen in a strong magnetic field and in zero field. The `Octave` program is presented in Appendix A. This is one case where the program is shorter than the tables it calculates and replaces. In zero-field with 30 radial points ( $N = 31$ , excluding excluding  $-1$  and  $1$  in the compactified domain, corresponding to the origin and infinity, respectively in the real domain) and with 12 angular points ( $M = 11$ ), it calculates the eigenvalues up to principal quantum number,  $n = 12$  to at least three digits of accuracy (a total of 650 states). Up to  $\beta \sim 10$  it determines the low-lying states of hydrogen (again with  $N = 31$  and  $M = 11$ ) to at least three digits of accuracy (Thirumalai & Heyl 2009; Ruder et al. 1994); for  $\beta \lesssim 1$ , the accuracy is typically two orders of magnitude better. The distinct advantage of the pseudospectral algorithm is the speed to achieve accurate results. The fine mesh calculations of Thirumalai & Heyl (2009) took up to two days or  $1.7 \times 10^5$  seconds — the pseudospectral algorithm takes about 1.4 s to get the same accuracy on the same processors. The algorithm uses spherical coordinates so it is not well suited to fields much stronger than  $\beta = 10$ . At  $\beta = 100$ , a finer mesh ( $M = 31$  and  $N = 51$ ) and 150 seconds of computation time are required to obtain three digits of agreement with Ruder et al. (1994); however, in this regime, cylindrical coordinates may be more appropriate and one can use the adiabatic approximation to obtain accurate results (Heyl & Hernquist 1998).

### 3.2 Helium and Lithium

The problem of multi-electron atoms (Appendix B) is of course much more complicated than hydrogen. Again we begin with the zero-field case, but we have many states to examine that test the direct and exchange interactions separately. In this case some validation for a vanishing magnetic field is useful. Table. 1 compares the zero-field results for some low-lying states of helium and lithium with the experimentally determined values from Ralchenko et al. (2008). Again the algorithm achieves typically better than one-percent accuracy rapidly.

Of course, the technique is not intended to supplant the popular, accurate and fast MCHF algorithms such as those of Fischer (1997). Such algorithms achieve their speed and

**Table 1.** Comparison of the observed zero-field states of helium and lithium from Ralchenko et al. (2008) to the values calculated here. Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge  $Zc$ , where  $Z = 2$  for helium and  $Z = 3$  for lithium. We use  $M = 7$ ,  $N = 31$  and  $r_Z = 58$ . The value of  $r_Z$  is chosen to provide close agreement for the ground state of helium and held fixed. Individual calculations take about ten seconds for helium and twenty for lithium. The primary source for the helium data is Drake & Martin (1998) and Moore (1971) for the lithium data.

Conf.	Term	$J$	$E_{\text{exp}}$	$E_{\text{spe}}$	$\Delta(\%)$
Helium I					
$1s^2$	$^1S$	0	1.451692958	1.43189	-1.364
$1s2s$	$^3S$	1	1.087514256	1.08996	0.225
$1s2s$	$^1S$	0	1.072885081	1.07929	0.598
$1s2p$	$^3P^o$	2	1.066484964	1.06856	0.195
		1	1.066484790	1.06857	0.196
		0	1.066482539	1.06856	0.195
$1s2p$	$^1P^o$	1	1.061818980	1.06593	0.387
		1	1.061818980	1.06594	0.388
$1s3s$	$^3S$	1	1.034248834	1.03719	0.284
$1s3s$	$^1S$	0	1.030539891	1.03456	0.391
$1s3p$	$^3P^o$	2	1.028945784	1.03174	0.272
		1	1.028945735	1.03174	0.271
		0	1.028945117	1.03174	0.272
$1s3d$	$^3D$	3	1.027722445	1.03073	0.293
		2	1.027722439	1.03073	0.293
		1	1.027722338	1.03073	0.293
$1s3d$	$^1D$	2	1.027714652	1.03073	0.294
$1s3p$	$^1P^o$	1	1.027476815	1.03092	0.335
Lithium I					
$1s^22s$	$^2S$	1/2	1.661773620	1.65595	-0.350
$1s^22p$	$^2P^o$	1/2	1.646683387	1.64097	-0.347
		3/2	1.646683042	1.64097	-0.347
$1s^23s$	$^2S$	1/2	1.634226909	1.62883	-0.330

accuracy by using the spherical symmetry of the atom: for example, by using spherical harmonics and a special treatment of full shells. The power of this pseudospectral algorithm becomes crucial when spherical symmetry is destroyed by a strong magnetic field.

Table 2 traces the binding energy of two low-lying states of helium using the software in Appendix B. The agreement with our earlier work (Thirumalai & Heyl 2009) is striking at weaker fields but as the magnetic field starts to dominate the atom, the agreement is poorer. Better agreement is achieved by increasing the angular resolution of the calculation to account for the changing shape of the atom.

For lithium we compare with the results of Al-Hujaj & Schmelcher (2004) who use a different parameter for the strength of the field,  $\gamma = 2Z^2\beta_Z = 18\beta_Z$  where the second equality holds for lithium. We have chosen to use eight angular grid points and thirty-two in the radial direction.

Here the agreement with the previous work is encouraging at least up to moderate field strengths ( $\gamma < 1$ ). For stronger fields the pseudospectral method typically yields excessively bound systems, except for the  $1^4(-3)^+$  state that happens to be the most bound state in strong magnetic fields. These spurious eigenvalues are not uncommon for pseudospectral methods (e.g. Boyd 2001). The software as presented in the appendices actually includes a filter for a blatantly spurious eigenfunction that attains a large value

**Table 2.** Table listing the binding energies of the most tightly bound states of helium in moderate to large magnetic fields;  $M_z = -1$  or  $M_z = -2$  and  $S_z = -1, \pi_z = +1$ . Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge  $Zc$ , where  $Z = 2$  for helium. The results from the current work can be compared readily with previous work (Thirumalai & Heyl 2009; Ruder et al. 1994). The first row for  $\beta_Z = 1$  is for  $M = 11$  like the other rows; the second row gives the results from  $M = 41$ . TH08 indicates results from Thirumalai & Heyl (2009), and R94 indicates results from Ruder et al. (1994).

$\beta_Z$	$M_z = -1$			$M_z = -2$		
	Here	TH08	R94	Here	TH08	R94
0.01	1.1221	1.1183	1.1182	1.0871	1.0852	1.0828
0.02	1.1656	1.1612	1.1609	1.1265	1.1234	1.1207
0.05	1.2734	1.2691	1.2658	1.2215	1.2175	1.2097
0.07	1.3359	1.3319	1.3258	1.2764	1.2732	1.2596
0.10	1.4211	1.4189	1.4069	1.3515	1.3510	1.3266
0.20	1.6586	1.6585	1.6270	1.5653	1.5598	1.5073
0.50	2.1603	2.1550	2.0508	2.0415	2.0009	1.8508
0.70	2.4584	2.4029	2.2329	2.2902	2.2246	1.9935
1.00	3.2165	2.7026	2.4675	3.0102	2.4981	2.2572
1.00	2.7115			2.6668		

**Table 3.** Table listing the binding energies of three tightly bound states of lithium in moderate to large magnetic fields. At the top of each pair of columns is the symmetry subspace  $2S+1(M_z)^z\text{-parity}$ . We take the dominant configuration for the ground state within each subspace. The column “Other” gives the values from Ralchenko et al. (2008) for zero field and from Al-Hujaj & Schmelcher (2004) elsewhere.

$\gamma$	$^20^+$		$^4(-1)^+$		$^4(-3)^+$	
	Here	Other	Here	Other	Here	Other
0.00	1.6560	1.6618	1.1968	1.1925	1.1358	1.1299
0.01	1.6590	1.6629	1.2017	1.1969	1.1427	1.1487
0.05	1.6681	1.6673	1.2192	—	1.1655	1.1663
0.10	1.6775	1.6705	1.2390	1.2334	1.1901	1.1869
0.20	1.6928	1.6741	1.2736	1.2674	1.2330	1.2278
0.50	1.7255	1.6729	1.3533	1.3463	1.3362	1.3294
1.00	1.8256	1.6575	1.4821	1.4432	1.4713	1.4627

along the magnetic axis for large distances from the nucleus. It is our experience with the hydrogen atom that these spurious eigenvalues become more prevalent for stronger magnetic fields and are more bound than the eigenvalues for well behaved eigenfunctions. However, the algorithm still finds the correct eigenvalue for the ground state, so with a more sophisticated filtering technique spurious eigenvalues can be eliminated for calculations in higher field strengths than considered here.

## 4 DISCUSSION

One of the primary goals of the current work was to provide a computational method that would be rather economical with regard to computation time, without having to compromise on accuracy. As can be seen in Table 1 the desired level of accuracy can be achieved with computation times on the order of seconds. The calculated values therein can conceivably have better agreement with experimentally determined values if effects of spin-orbit coupling, relativistic corrections and the effects of mixing of config-

urations were to be included. Similarly, upon examining Table 2, it is immediately apparent that the estimates of the binding energies of the state of helium corresponding to  $M_z = -1; S_z = -1$  are more bound than the previous estimates. The average improvement with respect to the values reported in our previous study (Thirumalai & Heyl 2009), is about 0.5% while, the average improvement over the values reported in Ruder et al. (1994) is about 3.4% over the entire range of magnetic field strengths reported therein. Similarly, upon comparing the results from the present calculation for the state of helium corresponding to  $M_z = -2; S_z = -1$  we see that they are more bound on average by about 1.5% and 5.8% respectively, with respect to the calculations of Thirumalai & Heyl (2009) and Ruder et al. (1994). Finally, when comparing with the results of other authors in Table 3 we see that the current single-configuration calculation using spectral methods provides binding energies that are an improvement on previous estimates for three tightly bound states of lithium. It can be seen that the average range of improvements for the estimates of the binding energies of the three states, relative to the calculations of other work, is about 1%.

In carrying out the calculations in the current study, as was noted earlier, the domain was compactified according to Eq. (4). This has the distinct advantage that one can set a boundary condition at true infinity rather than at a large value of the radial distance  $r$ . Typically, such a procedure renders the partial differential equations highly non-linear, making their solution with finite-element techniques more involved and computationally demanding, thus requiring a greater amount of computation time. In the current study, the compactification effectively changes the operators in Eqs. (6), (21) and (23).

Since the algorithm presented here is essentially a simple prototype, several avenues for further development are apparent. They address the stability, accuracy and robustness of the calculation. First from a physical point of view it does not make sense to use the same zoom radius (the value of  $r_Z$ ) for all of the electrons in an atom. The zoom radius is essentially the scale within which the radial mesh is fine; therefore, it should reflect the expected or calculated extent of the electronic wavefunctions. It would be quite natural to adaptively change the value of  $r_Z$  to be some constant factor times  $\langle r \rangle$  or  $\sqrt{\langle r^2 \rangle}$  as the Hartree-Fock iteration proceeds. Because the interelectron potential is smoother than the underlying wavefunctions it would be more effective to calculate the potentials for each electron using its own value of  $r_Z$  and then interpolate these results onto the meshes of the other electrons. In this manner the value of  $r_Z$  would adapt for the particular orbital that the electron occupies, achieving higher accuracy without increasing the number of radial mesh points. For the direct interaction this is straightforward because it is essentially a function; however, the exchange interaction is an operator or a matrix, as in Eq. (15), so the interpolation of the final result is a bit problematic. Rather it is expedient to interpolate the wavefunctions of the other electrons onto each other’s mesh and calculate the exchange interaction one pair at a time. Although this interpolation would necessarily make the code more cumbersome, it need not increase the processing time significantly. The inverse Laplacians for different values of  $r_Z$  are related to each other through simple scalings so the costly matrix

inversions would still only happen once at the beginning, and the results would scale for the appropriate values of  $r_Z$ .

A similar adaptation can be performed in the angular direction to focus grid points along the magnetic axis for strong magnetic fields. In this way we can achieve high accuracy for all of the electrons without including more grid points. A simple way to achieve this is the “Arctan/Tan” mapping (Boyd 2001) where the original angular variable  $\theta$  is mapped onto  $\theta'$  using

$$\theta' = \arctan(L \tan \theta) \quad (34)$$

The parameter  $L$  can change to reflect the actual physical extent of the wavefunction in the angular direction for each electron in the atom as the iterative process proceeds. This adaptation would add little additional overhead above the radial adaptive scheme outline in the last paragraph.

A second issue that we encountered is the appearance of spurious eigenvalues among the physical ones, especially for intense magnetic fields. The current software eliminates these eigenvalues by looking at the structure of the eigenfunctions. Essentially, many of the spurious eigenfunctions have significant support along the magnetic axis at large radii. Unfortunately, the current set of criteria are not sufficiently robust to exclude all of the spurious eigenfunctions. There are two clear paths to address this issue. The first is to develop a more sophisticated filtering technique to check the eigenfunctions during the iterative process. The second technique would be to use cylindrical coordinates that are better adapted to the intense-field limit where the wavefunctions essentially are well approximated by the product of Landau orbitals and a function of the coordinate along the magnetic field (the so-called adiabatic approximation). The use of cylindrical coordinates is of course not equivalent to the adiabatic approximation but it does fit better with the dominant symmetry of the intense-field problem. For this work we did not employ cylindrical coordinates because we wanted to verify our results against the zero-field limit where the binding energies of the various species are known precisely.

From a mathematical point of view, we have chosen to use Chebyshev points to sample in both the angular and radial directions. In this particular case it is possible to express the spectral derivatives using a fast-Fourier transform (Trefethen 2000; Boyd 2001). The most obvious application for the problem at hand would be to speed up the calculation of the direct component of the inter-electron potential; because this only makes a modest contribution to the workload, we decided to forgo the added complexity and use matrix multiplication to determine the inter-electron potential. On the other hand, given some additional work it may be possible to speed up other parts of the calculation using FFTs.

A final improvement would be to include several electronic configurations for each state (e.g. Al-Hujaj & Schmelcher 2004) not just the dominant one as we did here. Given the excellent agreement with the observed atomic properties that we found for the zero-field limit, we expect the improvement of a multi-configuration calculation to be modest at least for small atoms. However, recent theoretical results indicate that the atmospheres of neutron stars may be composed of elements near silicon (Hoffman & Heyl 2009), so including many configurations

may be crucial at least to verify the algorithm in the weak-field limit.

## 5 CONCLUSION

The amount of literature available regarding atoms in strong magnetic fields is quite extensive. Since the 1970s with improvements in both computing infrastructure and numerical methods the problem of atoms in strong magnetic fields has become increasingly tractable. However, the current state-of-the-art calculations still take on the order of hours if not days to obtain results of reasonable accuracy. To address this situation, we have, in this study, presented a new pseudospectral method for the calculation of the structure of atoms in strong magnetic fields. The key enabling advantages of the algorithm are its simplicity (about 130 lines of commented code) and its speed (about  $10^2 - 10^5$  times faster than finite-element methods to achieve similar accuracy). For hydrogen, helium and lithium it gives results that agree with the previous work at the few percent level or better for fields weaker than about  $2 \times 10^6$  T.

For the purpose of analyzing the spectra of magnetized white dwarfs and neutron stars it becomes crucial to have accurate data for the energy levels of different atoms in strong magnetic fields. With the ability to perform atomic structure calculations with a significant reduction in computation time, as with the pseudospectral methods described in this study, it becomes possible to amalgamate atomic structure calculation software with atmosphere models of neutron stars and white dwarf stars. This is a direct advantage of the software provided in the appendices to this paper. We have additionally presented several avenues for further research with the software including larger atoms, multi-configuration Hartree-Fock and full configuration-interaction calculations.

## ACKNOWLEDGMENTS

This research was supported by funding from NSERC. The calculations were performed on computing infrastructure purchased with funds from the Canadian Foundation for Innovation and the British Columbia Knowledge Development Fund. Correspondence and requests for materials should be addressed to [hey1@phas.ubc.ca](mailto:hey1@phas.ubc.ca). This research has made use of NASA's Astrophysics Data System Bibliographic Services

## REFERENCES

- Al-Hujaj O.-A., Schmelcher P., 2004, *Phys. Rev. A*, 70, 033411
- Boyd J. P., 2001, *Chebyshev and Fourier Spectral Methods*. Dover, Mineola
- Drake G. W. F., Martin W. C., 1998, *Canadian Journal of Physics*, 76, 679
- Fischer C. F., 1997, *Computational Atomic Structure, An MCHF Approach*. Institute of Physics Publishing, Bristol, UK
- Haines L. K., Roberts D. H., 1969, *Am. Journ. Phys.*, 37, 1145
- Heyl J. S., Hernquist L., 1998, *Phys. Rev. A*, 58, 3567
- Hoffman K. L., Heyl J. S., 2009, *MNRAS*, 400, 1986
- Loudon R., 1959, *Am. J. Phys.*, 27, 649
- Moore C. E., 1971, Technical Report 35, Atomic Energy Levels. Natl. Bur. Stand. (U. S.) Data Ser.
- Ralchenko Y., Kramida A. E., Reader J., Team N. A., 2008, Technical report, NIST Atomic Spectra Database (version 3.1.5). National Institute of Standards and Technology, Gaithersburg, MD.
- Ruder H., et al., 1994, *Atoms in Strong Magnetic Fields : Quantum Mechanical Treatment and Applications in Astrophysics and Quantum Chaos*. Springer-Verlag, New York
- Thirumalai A., Heyl J. S., 2009, *Phys. Rev. A*, 79, 12514 (16 pages)
- Trefethen L. N., 2000, *Spectral Methods in Matlab*. SIAM, p. 54

**APPENDIX A: MAGNETIZED HYDROGEN**

Both the single-electron and multiple-electron codes are self-contained Octave programs with the exception of the eight-line function `cheb` that Trefethen published previously in Trefethen (2000) and is available online at <http://www.comlab.ox.ac.uk/nick.trefethen/cheb.m>. This function calculates the differentiation matrix in Eq. (27). Both programs are also compatible with Matlab with some minor modifications in the output statements in the multi-electron program. However, after experimentation we concluded that the Octave version ran faster with our setup.

The hydrogen code is written as a function to be called from the Octave command line that returns the eigenfunctions, eigenvalues, angular and radial points, a list of the eigenfunctions that pass a rudimentary test and the “zoom” factor. For values of  $M$  and  $N$  on the order of ten, the vast majority of the computation time is devoted to calculating the eigenvalues, so the total execution time depends on the efficiency of the eigenvalue routine (`eig`); consequently, porting this algorithm to C does not result in a substantial speed up — in fact in our experience, Octave runs faster.

```
% HYDROGEN_S - calculate hydrogen in spherical coordinates
% beta is B/Bc, M is number of mu, N is number of radial
% the wavefunction is phi=f(r, mu=cos(theta))/r exp(i m phi)
% eigenfunctions in V, e-val in Lam, coords in (w,rs)
function [V,Lam,w,rs,igood,zoom] = hydrogen_s(beta,M,N,mphi)
% w coordinate, ranging from -1 to 1
[Dw,w] = cheb(M); D2w = Dw^2;
if (mphi~=0) w=w(2:M); Dw=Dw(2:M,2:M); D2w=D2w(2:M,2:M); end
Hw=-diag(1-w.*w)*D2w+diag(2.*w)*Dw;
% r coordinate, ranging from 1 to -1, rp from 1 to 0
[D,r] = cheb(N); rp = 0.5*(r+1); D = 2*D; D2 = D^2;
hh = diag(1-rp.*rp); D2 = hh*(hh*D2+diag(-2*r)*D); D = hh*D;
D2 = D2(2:N,2:N); D = D(2:N,2:N); rp = rp(2:N);
% zoom factor: set by coulomb and larmor radius; , rs from inf to 0
zoom=1/(1/110+sqrt(beta)/41); rs=zoom*atanh(rp); R = diag(1./rs); R2 = diag(1./(rs.*rs));
Hr=-1/(zoom*zoom)*D2-2*R; [rr,ww] = meshgrid(rs,w); rr = rr(:); ww = ww(:); rperp2=rr.*rr.*(1-ww.*ww);
if (mphi==0)
    H = kron(Hr,eye(M+1))+kron(R2,Hw)+diag(beta*beta*rperp2);
else
    H = kron(Hr,eye(M-1))+kron(R2,Hw)+diag(beta*beta*rperp2)+diag(mphi*mphi./rperp2);
end
[V,Lam] = eig(H); Lam = diag(Lam); [Lam,ii] = sort(Lam); Lam = Lam+2*beta*(mphi-1); V = V(:,ii);
% check outer B.C. and for bound states
igood = find((V(1,:).*V(1,:))'<(M*N)^(-2)*1e-4 & Lam<0);
```

**APPENDIX B: MAGNETIZED ATOMS**

The atomic code is written as a script to be called from the Octave command line because it has many parameters and diagnostics that one might like to examine and the script format encourages the user to choose what he or she wants to use.

Similar to the case of hydrogen, for values of  $M$  and  $N$  on the order of ten, the vast majority of the computation time is devoted to calculating the eigenvalues and inverting the Laplacians, so the total execution time depends on the efficiency of the eigenvalue and matrix inversion routines (`eig` and `inv`); consequently, we do not expect that porting this algorithm to a lower-level language (*e.g.* C) will result in a substantial speed up. In fact the computational effort is dominated by the diagonalization that is performed for each electron at each iteration. The inversion of the Laplacian is performed before the iterations begin.

```
% THREEDATOM - calculate an atom in three-D
% the wavefunction is phi=f(r,mu=cos(theta))/r
% r coordinate, ranging from -1 to 1
% Examples for Helium I
% nu=[1,1]; spin=[+1/2,-1/2]; mphi=[0, 0]; Z=2; %% 1s^2 1S J=0 : 1.43189
% nu=[1,2]; spin=[-1/2,-1/2]; mphi=[0, 0]; Z=2; %% 1s2s 3S J=1 : 1.08996
% nu=[1,2]; spin=[+1/2,-1/2]; mphi=[0, 0]; Z=2; %% 1s2s 1S J=0 : 1.07930
% nu=[1,1]; spin=[-1/2,-1/2]; mphi=[0,-1]; Z=2; %% 1s2p 3P0 J=2 : 1.06856
% nu=[1,3]; spin=[-1/2,-1/2]; mphi=[0, 0]; Z=2; %% 1s2p 3P0 J=1 : 1.06857
% nu=[1,1]; spin=[+1/2,+1/2]; mphi=[0,-1]; Z=2; %% 1s2p 3P0 J=0 : 1.06856
% nu=[1,1]; spin=[-1/2,+1/2]; mphi=[0,-1]; Z=2; %% 1s2p 1P0 J=1 : 1.06593
% nu=[1,3]; spin=[-1/2,+1/2]; mphi=[0, 0]; Z=2; %% 1s2p 1P0 J=1 : 1.06594
% Examples for Lithium I
```

```

nu=[1,1,2]; spin=[-1/2,+1/2,-1/2]; mphi=[0,0, 0]; Z=3; %% 1s^2 2s 2S J=1/2 : 1.65595
% nu=[1,1,3]; spin=[-1/2,+1/2,-1/2]; mphi=[0,0, 0]; Z=3; %% 1s^2 2p 2P0 J=1/2 : 1.64097
% nu=[1,1,1]; spin=[-1/2,+1/2,-1/2]; mphi=[0,0,-1]; Z=3; %% 1s^2 2p 2P0 J=3/2 : 1.64097
% nu=[1,1,4]; spin=[-1/2,+1/2,-1/2]; mphi=[0,0, 0]; Z=3; %% 1s^2 3s 2S J=1/2 : 1.62883
M=7; N=31; MAXITER=100; beta = 0;
% w coordinate, ranging from -1 to 1
[Dw,w] = cheb(M); D2w = Dw^2; Hw=-diag(1-w.*w)*D2w+diag(2.*w)*Dw;
% add zero weight to last term so we always use the same-sized vectors
w_w=[inv(Dw(1:M,1:M))(1,:),0];
% r coordinate, ranging from 1 to -1, rp from 1 to 0,
% rs from infinity to 0 (see below)
[D,r] = cheb(N); rp=0.5*(r+1); D = 2*D; D2 = D^2;
hh=diag(1-rp.*rp); D2=hh*(hh*D2+diag(-2*rp)*D);
wr=inv(D(1:N,1:N))(1,:);
% drop infinite weight at infinity (i.e. 1) since w.f. goes to zero quickly
% now wr is the same dimension as D2 etc.
wr=wr(2:N)./(1-rp(2:N).^2)';
% now multiply by hh so we didn't have zero for inversion above
D=hh*D;
% Radial Laplacian minus r=infinity (for potential calculations)
D2inf = D2(2:N+1,2:N+1);
% Construct Laplacian minus r=0 and r=infinity
% (set diricelet b.c. in radial direction for eigenvalue equations)
D2 = D2(2:N,2:N); D = D(2:N,2:N); rp=rp(2:N);
zoom=1/(1/116+sqrt(beta)/41)*0.5; rs=zoom*atanh(rp); wr=zoom*wr;
R = diag(1./rs); R2 = diag(1./(rs.*rs));
% Hamilton for radial coordinate
Hr=-1/(zoom*zoom)*D2-2*R;
[rr,ww] = meshgrid(rs,w); rr = rr(:); ww = ww(:); DIMEN=numel(rr);
rperp2=rr.*rr.*(1-ww.*ww); RR=diag(1./rr); we=2*pi*kron(wr,w_w);
% Full single electron Hamiltonian
H=kron(Hr,eye(M+1))+kron(R2,Hw)+diag(beta*beta*rperp2);
mmax=0;
for e1cnt=1:numel(mphi)-1
    for e2cnt=e1cnt+1:numel(mphi)
        if (spin(e1cnt)==spin(e2cnt))
            dum=abs(mphi(e1cnt)-mphi(e2cnt));
            if (dum>mmax) mmax=dum; end
        end
    end
end
% Construct Laplacians for electron potential calculation
Linv=zeros(DIMEN,DIMEN,mmax+1);
for i=0:mmax
% set the denominator equal to one, if it goes to zero (don't want an infinity)
% we will drop rperp2=0 later
L=kron(1/(zoom*zoom)*D2,eye(M+1))-kron(R2,Hw)-diag(i*i./(rperp2+(rperp2==0)));
% set the BC for rperp2=0 but add in identity so can be inverted
% an infinity in the last step would have given a NaN here
if (i~=0) L=diag(rperp2==0)+diag(rperp2~=0)*L*diag(rperp2~=0); end
% add in the origin as a single point
L=[ L, kron(D2inf(1:N-1,N),ones(M+1,1))]; kron(D2inf(N,1:N-1),ones(1,M+1)), D2inf(N,N)];
% invert Laplacian and set boundary condition at origin
Linvhold=(eye(DIMEN+1)-[zeros(DIMEN+1,DIMEN),ones(DIMEN+1,1)])*inv(L);
% divide by R before and after and remove origin!
% don't need to set B.C. again because the solutions for mphi~=0 are already zero in the
% right places, and the e-val equation sets them to zero when needed
Linv(:, :, i+1)=-4*pi*RR*Linvhold(1:DIMEN,1:DIMEN)*RR;
end
u=zeros(DIMEN,numel(nu));
direct_old=zeros(DIMEN,DIMEN,numel(nu));
exchange_old=zeros(DIMEN,DIMEN,numel(nu),mmax+1);

```

```

direct_new=zeros(DIMEN,DIMEN,numel(nu));
exchange_new=zeros(DIMEN,DIMEN,numel(nu),mmax+1);
interact=zeros(DIMEN,DIMEN);
% begin iterations
etotold=1e33; etot=1; j=1;
while (abs((etot-etotold)/etot)>1e-5 & j<MAXITER)
% calculate each electron wf
  etotold=etot;
  etot=0;
  for e1cnt=1:numel(nu)
    interact=zeros(DIMEN,DIMEN);
    for e2cnt=1:numel(nu)
      if (e2cnt~=e1cnt)
        if (spin(e1cnt)==spin(e2cnt))
          interact=interact+direct_old(:, :, e2cnt) ...
            -exchange_old(:, :, e2cnt,abs(mphi(e1cnt)-mphi(e2cnt))+1);
        else
          interact=interact+direct_old(:, :, e2cnt);
        end
      end
    end
  end
  if (mphi(e1cnt)==0)
    [V,Lam] = eig(H+2/Z*interact);
  else
    Htmp=H+2/Z*interact+diag(mphi(e1cnt)*mphi(e1cnt)./rperp2);
% apply boundary condition along z-axis, remove columns and rows with rperp2==0
    [V,Lam] = eig(reshape(Htmp(find(rperp2*rperp2'~=0)),(N-1)*(M-1),(N-1)*(M-1)));
    end
    Lam = diag(Lam); [Lam,ii] = sort(real(Lam));
    igood = find((V(1,:).*V(1,:))'<(M*N)^(-2)*1e-4);
    V = V(:,ii); uu=V(:,igood(nu(e1cnt)));
% add in boundary condition for angular direction (along z-axis), if needed
    if (mphi(e1cnt)~=0)
      uu=[zeros(1,N-1);reshape(uu,M-1,N-1);zeros(1,N-1)](:);
    end
    l(e1cnt)=Lam(igood(nu(e1cnt)))+2*beta*(mphi(e1cnt)+spin(e1cnt)-0.5);
    u2=uu.*uu; norm=we*u2; u2=u2/norm; uu=uu/sqrt(norm); u(:,e1cnt)=uu; % normalize
    eeen(e1cnt)=2/Z*we*(uu.*(interact*uu)); etot=etot+l(e1cnt)-eeen(e1cnt)/2;
    printf('J=%d e1=%d E-val: %18.12f EE: %18.12f Etot: %18.12f\n',j,e1cnt,l(e1cnt),eeen(e1cnt),etot);
    direct_new(:, :, e1cnt)=diag(Linv(:, :, 1)*u2);
    for i=1:mmax+1 exchange_new(:, :, e1cnt,i)=diag(uu)*Linv(:, :, i)*diag(uu); end
  end
  j=j+1; direct_old=direct_new; exchange_old=exchange_new;
end
if (j==MAXITER)
  printf('Did not converge\n');
end

```