

# Photoionization of hydrogen in white dwarf strength magnetic fields

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## Abstract

A new computational scheme, based on the complex-rotation method combined with a mixed Slater-Landau basis expansion, has been developed to calculate photoionization of atomic hydrogen in strong magnetic fields typical of magnetic white dwarf stars. Photoionization cross sections are presented for the ground and the  $2p$  excited states for selected magnetic field strengths and found to be in good agreement with available theoretical results. The current scheme is more efficient than previously reported methods as the basis expansion explicitly incorporates the physics of the strong-field regime. The method is particularly advantageous to quantitatively elucidate complex features of positive-energy spectra and to compute continuum absorption parameters for magnetic white dwarfs.

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Studies on the spectroscopy and dynamical behavior of atoms in a magnetic field have been pursued for many decades due to theoretical and experimental interests in the subject and the importance of practical applications in astrophysics and solid state physics. Especially, both the theoretical and application interests have been enhanced enormously after the discovery of strong magnetic fields in the atmospheres of white dwarf stars ( $10^2$  -  $10^5$  T) and neutron stars ( $10^7$  -  $10^9$  T) [1]. To date, a large number of studies have been devoted to the subject (see, e.g., [2–13]). As a magnetic field between  $10^2$  -  $10^9$  T is too strong to be realized in the laboratory, efforts have focused mainly on theoretical investigations. Several approaches, such as the Hartree-Fock [2, 3], finite-element [4], Kantorovich [5], variational [6], and power series expansion [7] methods have been developed to calculate the electronic structure of atoms [2–7] and radiative transition probabilities [8, 9] in various field strength regimes. The resulting atomic energy levels and radiative transition probabilities are essential to specification of bound discrete spectral lines, but is insufficient to elucidate positive-energy, or bound-free, spectra which are believed to provide significant continuum opacity in astronomical objects with strong magnetic fields. One needs bound-free transition theory to understand the complex features of positive-energy spectra.

One of the earliest bound-free studies was that reported by Alijah *et al.* [10] on photoionization cross sections of hydrogen in a magnetic field of 2000 T. They numerically solved coupled Schrödinger equations in combination with multichannel quantum defect theory. Later, Wang and Greene [11] developed a R-matrix method to investigate the problem. The complex-rotation method was also applied to such investigations by Delande *et al.* [12] and Merani *et al.* [13]. They selected a Sturmian basis set to expand eigenvectors of the rotated Hamiltonian  $H(\Theta)$ . The advantage of the Sturmian basis is that matrix elements of the Hamiltonian are of a known analytical form resulting in possible computational savings. The disadvantage is that a very large basis size is needed to obtain converged results. For example, Delande *et al.* and Merani *et al.* diagonalized a  $10000 \times 10000$  complex matrix to calculate photoionization cross sections of hydrogen with a magnetic field from 11700 to 23500 T (0.05 - 0.1 a.u.).

Based on the complex-rotation method, we develop a new computational scheme to calculate photoionization of hydrogen in a magnetic field. The mixed Slater-Landau basis proposed by Chen and Goldman [6] is adopted in this scheme. Because such a basis incorporates both limiting cases, corresponding to pure Coulomb states and pure Landau states,

with correct solutions at each limit, the basis size should be much smaller than the Sturmian basis size used in Refs. [12, 13]. Using this scheme, we have calculated photoionization cross sections of hydrogen in the ground state and the  $2p$  excited state with magnetic fields from 0.05 to 1.0 a.u.

The complex-rotation method was first introduced to compute photoionization cross sections by Rescigno and McKoy [14], and successfully applied to many atomic and molecular systems (see, e.g., [13, 15]). Details of the method can be found in Ref. [14]. Here we only outline its application to the current problem. The Hamiltonian of a hydrogenic atom in a uniform magnetic field  $B$  parallel to the quantization  $z$ -axis in atomic units is

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{B}{2}(\ell_z + \sigma_z) + \frac{B^2}{8}r^2 \sin^2 \theta, \quad (1)$$

where  $\ell_z$  and  $\sigma_z$  are the  $z$  components of the orbital and spin angular momenta, respectively. In the complex-rotation method, the radial coordinates are transformed by  $r \rightarrow re^{i\Theta}$ , where  $\Theta$  is the rotational angle. Therefore, the transformed Hamiltonian  $H(\Theta)$  is written in the form

$$H(\Theta) = -\frac{1}{2}\nabla^2 e^{-2i\Theta} - \frac{1}{r}e^{-i\Theta} + \frac{B}{2}(\ell_z + \sigma_z) + \frac{B^2}{8}r^2 \sin^2 \theta e^{2i\Theta}. \quad (2)$$

The mixed Slater-Landau basis set [6] has the form

$$\phi_{nl} = r^n (\cos \theta)^{\ell-|m|} (\sin \theta)^{|m|} e^{-\lambda r - \eta r^2 \sin^2 \theta} e^{im\phi}, \quad (3)$$

where  $m$  is the magnetic quantum number,  $n = 0, 1, 2, \dots, N_r$ ;  $\ell$  takes even or odd integer values greater than or equal to  $|m|$  up to  $N_\theta$ ; and  $\lambda$  and  $\eta$  are optimized nonlinear variational parameters related to the two limits, pure Coulomb states and pure Landau states. This basis is nonorthogonal. In such a basis set, the eigenvalue equation is expressed in matrix notation

$$H(\Theta)X(\Theta) = E(\Theta)NX(\Theta), \quad (4)$$

where  $N$  is the overlap matrix with nonzero matrix element  $N_{nl,n'\ell'} = \langle \phi_{nl} | \phi_{n'\ell'} \rangle$ . The complex eigenvalue problem cannot be solved simply by diagonalizing  $H(\Theta)$  due to the presence of the overlap matrix. A numerically stable procedure for the decomposition of the  $N$ -matrix is needed to solve Eq. (4). Cholesky decomposition was found to be successful [15], but requires that the matrix elements of  $N$  have a high precision when a basis size is large ( $N_r > \sim 20$ ). Here we adopt the singular value decomposition method [16]. Once

the overlap matrix is successfully decomposed, the solution is a simple problem of matrix diagonalization.

The photoionization cross section  $\sigma(\omega)$  is written as, from an initial state  $|\psi_0\rangle$  with energy  $E_0$  in atomic units [15],

$$\sigma(\omega) = 4\pi\alpha\omega \operatorname{Im} \sum_i \frac{\langle \bar{\psi}_i | R(\Theta) D | \psi_0 \rangle^2}{E_i - E_0 - \omega}, \quad (5)$$

where  $\alpha$  is the fine-structure constant,  $\omega$  the photon energy,  $D = \vec{e} \cdot \vec{r}$  the dipole-length operator with light polarization vector  $\vec{e}$ , and  $|\psi_i\rangle$  and  $E_i$  the complex eigenvector and eigenvalue of the rotated Hamiltonian  $H(\Theta)$ , respectively, obtained by solving Eq. (4).  $\langle \bar{\psi}_i |$  denotes the complex conjugate of the angular variables, but not of the radial variables of  $\langle \psi_i |$ , and  $R(\Theta)$  is the complex-rotation operator,

$$R(\Theta) = \exp\left(-\Theta \frac{\vec{r} \cdot \vec{p} + \vec{p} \cdot \vec{r}}{2}\right). \quad (6)$$

Using the basis set of Eq. (3), the eigenvalue problem is solved for the bound states  $n\ell_m$  of hydrogen in a magnetic field. For convenience, we solved the bound state problem with the same approach, but took the transformation angle  $\Theta = 0$ . We should point out that doing so is equivalent to diagonalizing the real matrix with the variational method. By adjusting the nonlinear optimizing parameters  $\lambda$  and  $\eta$ , one can obtain the most stable range of the variational energy eigenvalue and therefore the optimal energy eigenvalues are determined. The optimization of  $\lambda$  and  $\eta$  relies on their physical consideration. These two parameters are closely related to the two limits. In the Coulomb limit,  $\eta = 0$  and  $\lambda = 1$  for the ground state and  $\lambda = 1/n$  for the excited state with the principal quantum number  $n$ , while in the Landau limit,  $\eta = B/4$  [6]. Thus for non-zero, but finite  $B$ ,  $\lambda$  should vary between 0 and 1 (or  $1/n$ ) and  $\eta$  between 0 and  $B/4$ . Table I lists binding energies for the  $1s_0$  and  $2p_{-1}$  as a function of magnetic field with the current results compared to available calculations. An infinite proton mass was assumed and the spin quantum number  $m_s$  was taken to be  $-1/2$ . Excellent agreement can be seen between our binding energies and those from previous work. Adoption of 55 - 136 basis vectors, which correspond to 0.05 - 1.0 a.u. magnetic fields, results in more converged digits than reported by the other methods. In the whole calculation, quadruple precision is employed to guarantee computational accuracy.

To calculate the photoionization of hydrogen in a magnetic field, the transformation  $r \rightarrow r\Theta$  is applied to the Hamiltonian for the final continuum states. By adjusting the nonlinear

parameters  $\lambda$  and  $\eta$ , we obtain the wavefunctions and energy spectra of the continuum states. To test the current computational scheme, we first reproduce previously reported results [11–13]. Figures 1 (a) and (b) display photoionization cross sections for  $B = 0.1$  a.u. as a function of free electron energy. The ionization is from the hydrogen ground state  $1s_0$  to final states with  $\ell_z = 0$  and odd  $z$  parity, namely  $m^{\pi z} = 0^-$ , where  $\pi$  denotes parity. The light polarization is assumed to be along the magnetic field. The transformation angle used in all calculations of this paper is taken to be  $\Theta = 6^\circ$ . The arrows in this and later figures indicate the Landau thresholds. Figures 1 (a) and 1 (b) correspond, respectively, to  $N_r = 30$  and  $N_\theta = 29$  with a total basis size of 450, and  $N_r = 20$  and  $N_\theta = 19$  for a total basis size of 200.

The cross sections in Fig. 1 are in excellent agreement [17] with those presented by Delande *et al.* [12] and Wang and Greene [11] (see, *e.g.*, Fig. 2 of Ref. [12]). Although only 450 basis vectors are used in the current method, we obtained the same results as Ref. [12] where a  $10000 \times 10000$  matrix were diagonalized. From Figs. 1 (a) and 1 (b), one sees that the two cross sections are in good agreement for the first five resonances of each Landau threshold, but not for the later resonances. The comparison shows that 200 basis vectors are insufficient to describe the resonances close to the Landau thresholds. As the rotated continua are represented by a set of discrete eigenvalues in the complex-rotation method and imaginary parts of the discrete eigenvalues in close vicinity to the Landau threshold are very small, it is not possible to describe an infinite Rydberg series using a finite basis. Such basis set truncations are unavoidable in practical calculations [12]. Fortunately, the first several dominant resonances calculated with the truncated basis are stable, and thus sufficient to obtain the primary features of the positive-energy spectrum.

Figure 2 displays photoionization cross sections for a  $\Delta m = +1$  transition at  $B = 0.05$  a.u. from the excited  $2p_{-1}$  to final states with  $\ell_z = 0$  and even  $z$  parity, namely  $m^{\pi z} = 0^+$ . The calculations included  $N_r = 23$  and  $N_\theta = 22$  with a total basis size of 288. The same spectrum given in Fig. 2 was obtained by Merani *et al.*, but they used a basis of 10000 Sturmians. We find good agreement, but with a significantly reduced basis. Figures 3 (a) and 3 (b) display cross sections for  $B = 1.0$  and  $0.5$  a.u., respectively, which are presented here for the first time. We took  $N_r = 24$  and  $N_\theta = 23$  for a total basis size of 288 for  $B = 1.0$  a.u. and  $N_r = 20$  and  $N_\theta = 19$  with a total basis size of 200 for  $B = 0.5$  a.u.

In conclusion, we have developed a new computational scheme, based on the complex-

rotation method combined with a mixed Slater-Landau basis expansion, to calculate photoionization of hydrogen in a strong magnetic field. The scheme is found to be reliable by comparison with published photoionization cross sections, is shown to be more efficient than previously reported methods due to the utilization of significantly smaller basis sets, but can still quantitatively elucidate complex features of the positive-energy spectra. The method should prove to be useful for producing large sets of magnetic-field-dependent bound-free cross sections useful for the modeling of magnetic white dwarfs. Photoionization calculations for other excited states are in progress.

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- [1] R. H. Garstang, Rep. Prog. Phys. **40**, 105 (1977).
  - [2] M. V. Ivanov, J. Phys. B **21**, 447 (1988); **27**, 4513 (1994).
  - [3] W. Rösner, G. Wunner, H. Herold, and H. Ruder, J. Phys. B **17**, 29 (1984).
  - [4] J. Shertzer, Phys. Rev. A **39**, 3833 (1989).
  - [5] M. G. Dimova, M. S. Kaschiev, and S. I. Vinitzky, J. Phys. B **38**, 2337 (2005).
  - [6] Z. Chen and S. P. Goldman, Phys. Rev. A **45**, 1722 (1992).
  - [7] Yu. P. Kravchenko, M. A. Liberman, and B. Johansson, Phys. Rev. A **54**, 287 (1996).
  - [8] H. Forster, W. Strupat, W. Rösner, G. Wunner, H. Ruder, and H. Herold, J. Phys. B **17** 1301 (1984).
  - [9] W. Becken and P. Schmelcher, Phys. Rev. A **65**, 033416 (2002).
  - [10] A. Alijah, J. Hinze, and J. T. Broad, J. Phys. B **23**, 45 (1984).
  - [11] Q. Wang and C. H. Greene, Phys. Rev. A **44**, 7448 (1991).
  - [12] D. Delande, A. Bommier, and J. C. Gay, Phys. Rev. Lett. **66**, 141 (1991).
  - [13] N. Merani, J. Main, and G. Wunner, Astron. Astrophys. **298**, 193 (1995).
  - [14] T. N. Rescigno and V. McKoy, Phys. Rev. A **12**, 522 (1975).
  - [15] L. B. Zhao and Y. K. Ho, Phys. Plasmas **11**, 1695 (2004).
  - [16] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in*

TABLE I: Comparison of binding energies of states  $n\ell_m$  as a function of magnetic fields.

B (a.u.)	$E(1s_0)$ (a.u.)		$E(2p_{-1})$ (a.u.)	
	This work	others	This work	others
0.05	0.52437670670614178	0.524376706706 <sup>a</sup>	0.168058188453778	0.168058188454 <sup>a</sup>
0.1	0.54752648040109449	0.547526480401 <sup>a</sup>	0.200845672373340	0.200845672373 <sup>a</sup>
		0.5475265 <sup>b</sup>		0.2008457 <sup>b</sup>
		0.5475264804010945 <sup>c</sup>		0.20084567237333 <sup>c</sup>
0.5	0.69721053845807936	0.697210538458 <sup>a</sup>	0.349477297763186	0.349477297763 <sup>a</sup>
		0.6972105384 <sup>d</sup>		0.3494772977 <sup>d</sup>
1.0	0.83116889673315803	0.831168896733 <sup>a</sup>	0.456597058423752	0.456597058424 <sup>a</sup>
		0.831169 <sup>b</sup>		0.4565971 <sup>b</sup>
		0.83116889673 <sup>c</sup>		0.4565970584 <sup>c</sup>

<sup>a</sup>Ref. [7]; <sup>b</sup>Ref. [3]; <sup>c</sup>Ref. [6]; <sup>d</sup>Ref. [5].

*FORTTRAN*, 2nd. ed. (Cambridge University Press, Cambridge, 1992)

[17] Note to the editor and referees: We attempted to contact the authors of Refs. [11-13] to obtain their numerical results to make comparative plots, but they either did not have the data or failed to respond.

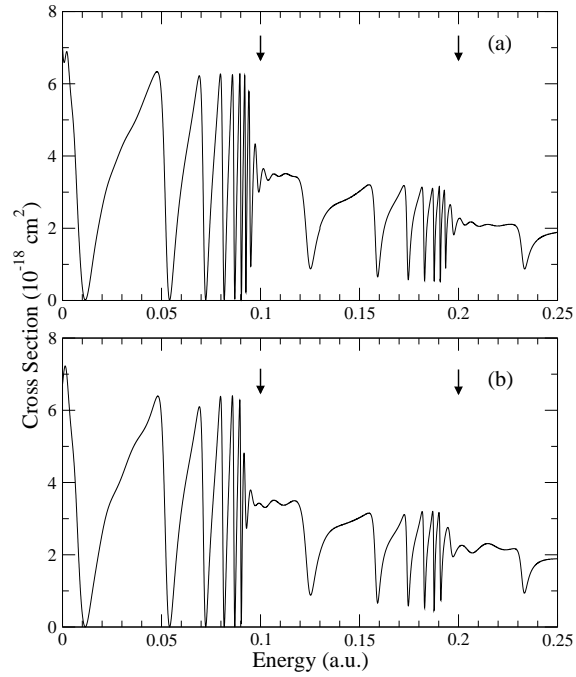


FIG. 1: Cross sections of hydrogen in a magnetic field of  $B = 0.1$  a.u. as a function of the free electron energy. The photoionization is from the ground state  $1s_0$  to final states with  $\ell_z = 0$  and odd  $z$  parity. (a) and (b) are calculated with 450 and 200 basis vectors, respectively. Note that the energy scale includes the contribution from the spin term in Eq. (1).

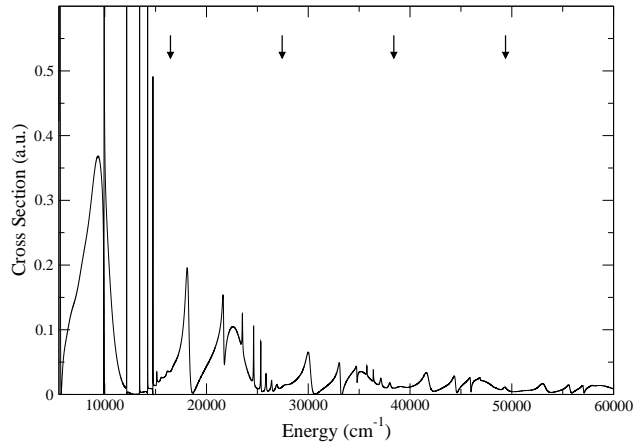


FIG. 2: Cross sections for  $\Delta m = +1$  bound-free transitions of hydrogen in a magnetic field of  $B = 0.05$  a.u. as a function of the free electron energy. The photoionization is from the excited state  $2p_{-1}$  to final states with  $\ell_z = 0$  and even  $z$  parity. 288 basis vectors were included in the calculation. Note that the energy scale neglects the spin term to facilitate direct comparison with the results of Merani *et al.* [13].

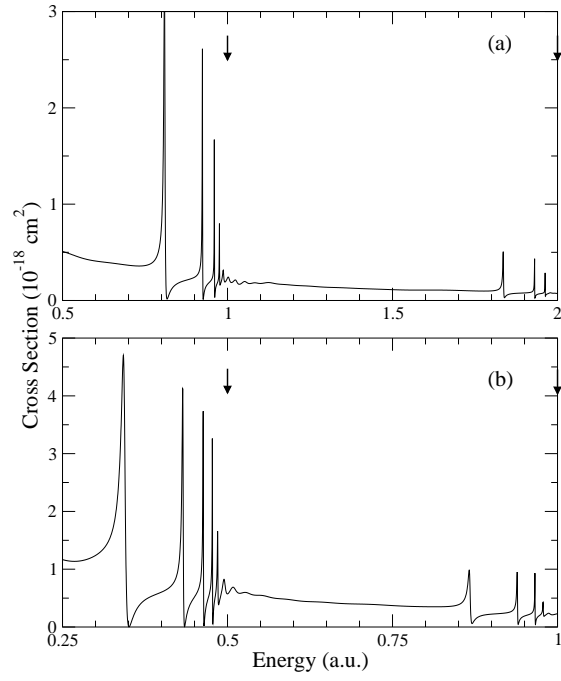


FIG. 3: Same as Fig. 1, but (a)  $B = 1.0$  a.u. with 288 basis vectors and (b)  $B = 0.5$  a.u. with 200 basis vectors.