Hartree-Fock calculations for the photoionisation of helium and helium-like ions in neutron star magnetic fields

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We derive the photoionisation cross section in dipole approximation for many-electron atoms and ions for neutron star magnetic field strengths in the range of \(10^7\) to \(10^9\) T. Both bound and continuum states are treated in adiabatic approximation in a self-consistent way. Bound states are calculated by solving the Hartree-Fock-Roothaan equations using finite-element and B-spline techniques while the continuum orbital is calculated by direct integration of the Hartree-Fock equations in the mean-field potential of the remaining bound orbitals. We take into account mass and photon density in the neutron star’s atmosphere as well as thermal occupation of the levels. The data are of importance for the quantitative interpretation of observed x-ray spectra that originate from the thermal emission of isolated neutron stars. They can serve as input for modeling neutron star atmospheres as regards chemical composition, magnetic field strength, temperature, and redshift. Our main focus in this paper lies on helium, helium-like oxygen and helium-like iron. These two-electron systems are simple enough to calculate all possible transitions when limiting the quantum numbers and should show all the basic structures and behaviour of other two-electron systems up to iron.

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I. INTRODUCTION

Atoms in neutron star magnetic fields have been the subject of research for almost 40 years, starting with the analysis of the simplest chemical element, the hydrogen atom. A historical review of the work on the hydrogen atom in strong magnetic fields can be found in the book by Ruder et al. [1]. In particular, in the early 1980’s bound-bound [1] as well as bound-free [2] transitions of hydrogen in strong magnetic fields were calculated.

Studies of heavier elements have received renewed impetus from the discovery of broad absorption features in the thermal X-ray emission spectra of the isolated neutron star 1E 1207.4-5209 [3, 4] and three other isolated neutron stars [4, 8] by the Chandra X-Ray Observatory by NASA and the XMM-Newton Observatory by ESA. These features could be of atomic origin [9-11]. As can be seen from the review article on neutron star thermal emission by Zavlin [12], magnetized models of neutron star atmospheres have largely been confined to hydrogen atmospheres, partially or fully ionised. The only attempt in the literature to model magnetized heavy element (carbon, oxygen, neon) atmospheres was undertaken by Mori and Ho [13]. They showed that the features observed in 1E 1207 could be due to transitions of oxygen in different ionisation stages. Pavlov and Bezchastnov [14] suggested that the features can be produced by bound-bound transitions of singly ionised helium in strong magnetic fields. A further interpretation in terms of peaks in the energy dependence of the free-free opacity has been put forward by Suleimanov et al. [15], but again there modelling is restricted to hydrogen atmospheres.

In view of the unknown chemical compositions of the atmospheres of neutron stars, any possible fusion product, i.e., all elements from hydrogen to iron in various ionisation stages, could produce features in the thermal emission spectra of neutron stars. In order to be in a position to calculate synthetic spectra for models of neutron star atmospheres and to compare with observed spectra, in principle a complete knowledge of both the bound-bound transitions and the bound-free transitions of all these elements in strong magnetic fields, and in all ionisation stages, would be required. While bound-bound transitions in many-electron systems in neutron star magnetic field strengths have already been investigated in the literature [16], calculations of photoionisation cross sections are few. Medin, Lai, and Potekhin [17] calculated a small number of bound-free transitions for helium in strong magnetic fields, as did Mori and Hailey [11] for oxygen and neon ions.

We wish to extend these calculations by performing a systematic and complete study of the total photoionisation cross sections of two-electron atoms for the physically realistic situation that the initial bound states are thermally occupied, and the atoms are exposed to black body radiation of the same temperature. As in [17] we work with the adiabatic approximation [18, 19] which implies that all electrons are in the lowest Landau level \((n = 0)\), with different magnetic quantum numbers \((m = 0, -1, -2, -3, \ldots)\), and the parts of the wave functions along the magnetic field are calculated self-consistently. (Adiabatic means, intuitively speaking, that the motion of the electrons in the plane perpendicular to the field is fast compared to the motion along the field, in which the electrons only feel the Coulomb potential of the nucleus, averaged over Landau orbitals.)

The specific difficulty in calculating photoionisation cross sections of many-electron atoms in strong magnetic fields is that the features can be produced by bound-bound transitions of singly ionised helium in strong magnetic fields...
fields lies in the lacking shell structure of these atoms. For every magnetic quantum number possible in the lowest Landau level there exists an energetically strongly lowered ground state (tightly bound state), while the energies of the excited states for every \( m \) form a Rydberg series (hydrogen-like states). Thus all excited states are practically \( m \)-degenerate, and, assuming thermal occupation of the initial states, occupied with equal probability. The summation of the individual cross sections for the ionisation of the atoms from the \( m \)-degenerate states by photons of given energy would therefore diverge. We will introduce a physically reasonable cut-off criterion to avoid the divergence.

The organisation of the paper is as follows: In Sec. \( \text{II} \) we briefly recapitulate the properties of atoms in intense magnetic fields and the Hartree-Fock-Finite-Elements Roothaan (HFFER) method used to determine the bound initial states. The orbitals of the resulting ion and of the continuum electron after the photoionisation are calculated separately and then combined to a Slater determinant characterising the final state. The cross sections are derived in Sec. \( \text{III} \). Atomic data for helium, helium-like oxygen and helium-like iron are presented in Sec. \( \text{IV} \). The influence of photon and mass density, and the longitudinal wave functions are expanded in terms of \( B \)-splines. The \( B \)-spline expansion coefficients are determined by minimising the total energy functional (for computational details of this HFFER method cf. \[20, 21\]).

### II. ATOMS IN VERY STRONG MAGNETIC FIELDS

For the readers' convenience we briefly review the basics of atoms in strong magnetic fields \[1\]. A magnetic field \( B \) is called strong if it exceeds the characteristic field strength \( B_0 = 4.70108 \times 10^5 \) T, i.e., when the magnetic field parameter \( \beta = B/B_0 \) is large. In our calculations we will concentrate on a magnetic field strength of \( B = 10^8 \) T which corresponds to \( \beta \approx 212 \). At \( B_0 \) the Larmor radius \( a_L \) becomes equal to the Bohr radius \( a_0 \). We note that \( a_L = a_0/\sqrt{\beta} \).

In strong fields the cylindrical symmetry of the magnetic field dominates, and it is therefore appropriate to work in cylindrical coordinates (we assume the field to point in the \( z \) direction). Then we can write the Hamiltonian for an \( N \)-electron atom or ion with nuclear charge \( Z \) (in atomic Rydberg units, i.e., \( \hbar = 4\pi\varepsilon_0 = 2m_e = e^2/2 \equiv 1 \)) in the form \( H = \sum_i \hat{H}_i \), with

\[
\hat{H}_i = -\left( \frac{\partial^2}{\partial \rho_i^2} + \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} + \frac{1}{\rho_i^2} \frac{\partial^2}{\partial \phi_i^2} + \frac{\partial^2}{\partial z_i^2} \right) - 2i \beta \frac{\partial}{\partial \phi_i} + \beta^2 \rho_i^2 \frac{1}{2} Z \right) + \frac{\beta^2}{\rho_i^2} + \frac{2 \beta}{\rho_i} \frac{z_i}{|\rho_i|} \right) + \sum_{j \neq i} \frac{2}{|r_i - r_j|} 1 \right)
\]

being the Hamiltonian for the \( i \)-th electron. In \( \text{I} \) \( \sigma_z \) is the \( z \) Pauli-matrix, and the term describes the interaction of the spin moment with the external field. At the magnetic field strength we consider, \( B = 10^8 \) T, the spin flip energy, which is also the Landau excitation energy, amounts to 11.6 keV, which is much larger than any single-orbital energy that we will encounter. Therefore it is justified to assume all electron spins to be aligned antiparallel to the magnetic field, and all single-electron states to occupy the lowest Landau level \( n = 0 \). The spin part of the state will be omitted in what follows.

The single-particle orbital of electron \( i \) is given by

\[
\Psi_i(\rho, \phi, z) = \Phi_{m_i}(\rho, \phi) g_{m_i, \nu_i}(z),
\]

where \( \Phi_{m_i}(\rho, \phi) \) is the lowest Landau orbital, with magnetic quantum number \( m_i \), and \( g_{m_i, \nu_i}(z) \) denotes the longitudinal part of the wave function. The quantum number \( \nu_i \) counts the number of nodes of the wave function along the \( z \) direction. In the following, states with quantum numbers \( m \) and \( \nu \) will be denoted by \((m, \nu)\). Recall that in the lowest Landau level \( m \) only assumes nonpositive values, \( m = 0, -1, -2, -3, \ldots \).

From the single-electron orbitals \( \text{II} \) of the bound electrons a Slater determinant is constructed, and the wave functions \( g_{m, \nu}(z) \) are determined self-consistently by solving the resulting Hartree-Fock equations. In our calculations, the \( z \) axis is divided into finite elements, and the longitudinal wave functions are expanded in terms of \( B \)-splines. The \( B \)-spline expansion coefficients are determined by minimising the total energy functional (for computational details of this HFFER method cf. \[20, 21\]).

The final state of the bound-free transition consists of the ionised core and the electron which is photoionised into the continuum. Near the atomic core the unbound electron is influenced by the bound electrons, while the bound electrons can be assumed to be unaffected by the unbound electron \( \text{I} \). Therefore the initial state of the atom and the bound part of the final state, i.e., the ionised core, can be calculated separately in advance by the above mentioned method.

The wave function of the continuum electron is calculated by solving the Hartree-Fock equations that result from its interaction with the electrons of the remaining core:

\[
\left[ -\frac{\partial^2}{\partial z^2} + V_m(z) + \sum_{j=1}^{N-1} \int d\zeta g_{m, \nu_j}(\zeta')U_{m, \nu_j}(z, \zeta') \right] g_{m, \nu}(z) = \epsilon' g_{m, \nu}(z).
\]

Here \( V_m(z) \) represents the effective electron-core potential, \( U_{m, \nu}(z) \) and \( A_{m, \nu}(z) \) denote the effective electron-electron potential and the exchange potential, respectively. The energy \( \epsilon' \) replaces the number of nodes \( \nu \) and is characteristic of the unbound electron. These three potentials can be computed numerically by evaluating the integrals.
\[ V_m(z) = -2Z \int \frac{\Phi_m(r)}{|r|} \, dr_z, \]
\[ U_{mm'}(z, z') = 2 \int \int \frac{\Phi_m(r) \Phi_{m'}(r')}{|r' - r|} \, dr_z \, dr_{z'}, \]
\[ A_{mm'}(z, z') = 2 \int \int \frac{\Phi_{m'}^*(r) \Phi_m(r) \Phi_{m'}^*(r') \Phi_{m'}(r')}{|r' - r|} \, dr_z \, dr_{z'}. \]

A detailed description of the evaluation of the above integrals can be found in [22].

The Hartree-Fock equations (3) are solved, for every given value of the continuum energy \( E' \), using a standard Runge-Kutta integrator. Since the \( z \) parity is a good quantum number, one can calculate a symmetric and an antisymmetric wave function by imposing corresponding initial conditions at \( z = 0 \). For \( z \to \pm \infty \) these wave functions assume a sinusoidal shape, close to the nucleus both the amplitude and the period decrease due to the interaction with the ionic core and the bound electrons. Because of the delocalised nature of the continuum wave functions they can be normalised only over a finite periodicity length \( d_z \). The latter, however, does not enter into the final results.

### III. CROSS SECTION FOR THE PHOTOIONISATION

In this section we give the formula for the photoionisation for the case that both the initial state \( \psi_1 \) and final state \( \psi_f \) are Slater determinants. The former is composed of \( N \) bound states, the latter consists of \( N - 1 \) bound and one unbound wave function. The Hamiltonian \( H_{\text{int}} \) for the interaction of the electrons with the radiation field \( A_\ell \propto e^{ikr} \) of the incoming photon is obtained by the usual minimal substitution of the momenta, \( p_i \to \pi_i = p_i - \sqrt{2}A_\ell \) (recall that in atomic Rydberg units \( e = \sqrt{2} \)), and by taking into account the interaction of the spin magnetic moments of the electrons with the magnetic field \( B_0 \), \( \nabla \times A_\ell \) of the radiation field:

\[ \hat{H}_{\text{int}} = \sum_{i=1}^{N} \left( 2\beta_i \hat{\sigma}_i - 2\sqrt{2} A_\ell \pi_i \right). \] (4)

In [11], \( \beta_i = B_i / B_0 \), and since we are interested in one-photon transitions the term quadratic in the vector potential has been omitted. The (one-dimensional) density of final states of the emitted (spin-down) electron is given by

\[ \rho_f = \frac{d_z}{2\pi} \sqrt{\frac{1}{4E'}}. \]

where \( d_z \) denotes the periodicity length in \( z \)-direction.

Starting from Fermi’s golden rule for the transition rate

\[ w(\Psi_f, \Psi_i) = 2\pi |\langle \Psi_f | H_{\text{int}} | \Psi_i \rangle|^2 \rho_f, \]

we can calculate the cross section by the usual relation \( w = j\sigma \), with \( j = c/V \) the photon flux of the incident radiation. Noting that in atomic Rydberg units \( c = 2/\alpha \), where \( \alpha \) is the fine-structure constant, we have the relation \( \sigma = \frac{V_o}{2\pi}w. \)

We calculate the photoionisation cross sections in dipole approximation. Therefore there are three types of transitions, which differ in the change of the total angular momentum in \( z \) direction (quantum number \( m = \sum m_i \)) caused by the absorption of the photon. Linearly, right, and left circularly polarised light induces transitions, with \( \Delta M = 0 \) (\( \sigma_0 \)), \( \Delta M = +1 \) (\( \sigma_+ \)) and \( \Delta M = -1 \) (\( \sigma_- \)), respectively.

Calculations in adiabatic approximation yield no transitions for left and right circularly polarised light when using the so-called ‘velocity form’ [23]. Consequently we switch from the ‘velocity form’ to the ‘length form’ using the well known commutator relation

\[ [\hat{H}_i, \pi_i] = -2i\sigma_i, \]

where \( \hat{H}_i \) designates the non-interaction-Hamiltonian of the \( i \)-th electron, cf. [11].

Lengthy but straightforward calculations finally yield the following explicit expressions for the photoionisation cross sections of the three types of dipole transitions:
wave function is shown in Fig. 4 for both parities for the final state \((m = 0, E' = 0.1 \, \text{eV})\) \((m = -199, \nu = 0)\), i.e., slightly above the ionisation threshold. For the symmetric function the first zero crossing occurs at about 0.2 \(a_0\), with \(a_0\) the Bohr radius. The zero crossing of the antisymmetric function is near 1.2 \(a_0\). The difference in the positions of the first node strongly affects the integrals in the cross section 5, and leads to quite different behavior of single cross sections with increasing transition energies.

**IV. CROSS SECTIONS OF TWO-ELECTRON SYSTEMS**

For reasons of simplicity we choose helium, helium-like oxygen and helium-like iron to be the systems of interest, because they are still simple enough to compute a huge amount of cross sections in reasonable time, and is complex enough to draw conclusions for other elements.

A. Single Cross Section

The behavior of single cross sections is mainly determined by the unbound wave function. Since \(z\)-parity is a good quantum number the wave function is either symmetric or antisymmetric. An example of a continuum
0, \( E' \) (\( m_4 = -199, \nu_4 = 0 \)) and (\( m_1 = 0, \nu_1 = 0 \)) (\( m_2 = -199, \nu_2 = 0 \)) \( \rightarrow \) (\( m_3 = 0, E' \)) (\( m_4 = -199, \nu_4 = 1 \)). Note that in the second transition, the quantum number \( \nu \) changes from 0 to 1, and therefore also the z-parity changes.

For two-electron atoms the double sum in [5] reduces to four possible terms, two with the continuum wave function in the dipole matrix element, and two with the continuum wave function in the minor:

\[
\begin{align*}
\langle g_{m_3 E'} | z_1 | g_{m_1 \nu_1} \rangle & \delta_{m_3, m_1} a_1^6 \\
+ \langle g_{m_3 E'} | z_2 | g_{m_2 \nu_2} \rangle & \delta_{m_3, m_2} a_2^6 \\
+ \langle g_{m_4 \nu_4} | z_1 | g_{m_1 \nu_1} \rangle & \delta_{m_4, m_1} a_4^2 \\
+ \langle g_{m_4 \nu_4} | z_2 | g_{m_2 \nu_2} \rangle & \delta_{m_4, m_2} a_4^2 
\end{align*}
\]

(6)

In the transitions considered both single-particle orbitals of the initial state are symmetric. Therefore, if the continuum wave function appears in the minor, as is the case for the last two terms in [5], the latter has a value different from zero only for the symmetric continuum wave function. On the other hand, does the continuum wave function appear in the dipole matrix element, as is the case for the first two terms in [5], only the antisymmetric continuum wave function yields a nonvanishing contribution because of the antisymmetry of the operator \( z \).

In the first transition considered only the term \( \langle g_{199 E'} | z | g_{00} \rangle \langle g_{-199 0} | \rangle \) contributes, and thus the antisymmetric continuum wave function, whereas in the second transition only the term \( \langle g_{-199 1} | z | g_{-199 0} \rangle \langle g_{0 E'} | \rangle \), and therefore the symmetric continuum wave function. The resulting cross sections are shown in Fig. 2 for helium at \( B = 10^8 \) T, and a photon incident perpendicular to the direction of the field.

![Fig. 2.](image)

**FIG. 2.** (Color online) Cross section for the photoionisation of helium from the initial state (\( m_1 = 0, \nu_1 = 0 \)) (\( m_2 = -199, \nu_2 = 0 \)) to the final states (\( 0, E' \)) (\( -199, 0 \)) (left) and (\( 0, E' \)) (\( -199, 1 \)) (right) as a function of the photon energy. The magnetic field strength is \( B = 10^8 \) T (\( \beta \approx 212 \)) and the photon is assumed to propagate perpendicular to the direction of the field.

The cross section of the first transition starts at the ionisation threshold 393.4 eV with a value of around \( 3 \times 10^6 a_1^6 \) and drops monotonously with rising transition energy. The second cross section with an ionisation threshold of 413.5 eV is smaller by four orders of magnitude and drops to zero several times, which is caused by zero crossings of the dipole matrix element. The reason for the different sizes of the cross sections is the \( z \)-parity of the unbound electron. The symmetric continuum wave function has its first node still close to the nucleus, therefore the overlap integral \( \langle g_{199 E'} | g_{00} \rangle \) contains positive and negative contributions of roughly the same size. By contrast, in the first transition the antisymmetric continuum wave function contributes, which has its first node further away from the nucleus, where the bound state appearing in the dipole matrix element has almost dropped to zero.

The cross sections of the same two transitions for Helike iron at different magnetic field strengths are shown in Fig. 3. We clearly see that the general behavior remains the same: The cross section of the first transition is much larger, and there are no zero crossings of the dipole matrix element in the energy range considered. For both transitions, the ionisation threshold rises with higher magnetic field strengths, but the curves are quite similar.

![Fig. 3.](image)

**FIG. 3.** (Color online) As Fig. 2 but for helium-like iron. The cross sections correspond, from left to right, to the magnetic field strengths \( \beta \approx 212, 500, 1000 \) and 2000.

We can conclude that, for stronger magnetic fields and higher nuclear charges, the only significant change is that the ionisation threshold is shifted to larger energies.

**B. Total Cross Section**

We now wish to calculate the total cross section for the ionisation by a photon of a given energy, which is the sum over all single cross sections \( \sigma = \sum_i \sigma_i \). Since in the lowest Landau level the magnetic quantum numbers in principle are not bounded below, this sum would diverge. To find a physically reasonable fact we make use of the fact that the spatial extension \( \rho_0 \) of a Landau state \( \Phi_{m\sigma}(\rho, \phi) \) is determined as [24]

\[
\rho_0^2 = a_L^2 \left( |m| + \frac{1}{2} \right)
\]

(7)

with \( a_L = a_0 / \sqrt{\beta} \) the Larmor radius. This means that as \( |m| \) increases the atoms become broader and broader in
the direction perpendicular to the field until, at a given mass density, for some \(|m| \) they begin to "touch" each other. This determines the maximum magnetic quantum number that has to be considered when summing for the total cross section. In the results presented below we chose a maximum value of \(|m| = 200\). In an analogous fashion we restrict ourselves to longitudinal wave functions with a maximum number of nodes \(\nu = 2\), since for larger number of nodes the orbitals would overlap at a given mass density. In Section V we will give values for the mass densities that are covered by these restrictions.

We note that with this the number of initial states amounts 180,300. Starting from these states, every possible transition has to be found. For every polarisation, these states lead in total to roughly 1 million transitions. In Fig. 4 we compare the total cross section of helium, summed over all possible ionisation processes, and helium-like oxygen.

![Figure 4](image_url)

**FIG. 4.** (Color online) Left: Total cross section for the photoionisation of helium at \(B = 10^8\) T obtained by summing over all initial states with \(|m| \leq 200\) and \(\nu \leq 2\) as a function of the photon energy for the three different polarisations. Right: The corresponding cross section for helium-like oxygen.

In both cases, the cross sections with circularly polarized light are several orders of magnitude smaller than the cross section with linearly polarised light. Also the general behavior of the curves for both elements is similar. The main difference is the position of the maximum cross section. As can be expected, the maximum for oxygen is at higher energies, due to the higher binding energy. The second difference is the absolute value, which is smaller for oxygen.

V. CROSS SECTION FOR REALISTIC PHYSICAL CONDITIONS OF A NEUTRON STAR

In this section we calculate effective photoionisation cross sections by taking into account the physical conditions that prevail in the neutron star atmosphere. First we assume a thermal occupation of the initial states and calculate total cross sections as a function of photon energy. Then we determine cross sections averaged over the photon energies of a Planckian spectrum. Finally we explore the effects of the plasma density and estimate the values for the mass density for which the cut-off criteria are valid.

A. Thermal occupation probability

Neutron star atmospheres are hot, with temperatures up to \(10^6\) K [12]. We account for this fact by a thermal occupation of the initial states, and in summing the single photoionisation cross sections weight their contributions to the total cross section according to their occupation probability \(p(E) = e^{-\Delta E/kT}\). From [11] and [22] we adopt a representative value of \(kT = 150\) eV and, to demonstrate the influence of an increase of temperature, of \(kT = 300\) eV.

The resulting cross sections are shown in Fig. 5. At higher temperatures the occupation probabilities of the excited bound states are larger, which yields an increase of the total cross section. Also, without thermal occupation weighting the cross section was much larger. We have the effect that single cross sections of excited initial states which manifested themselves at lower energies can be rather large, but are suppressed if thermal occupation probability is taken into account.

![Figure 5](image_url)

**FIG. 5.** (Color online) Total cross section for the photoionisation of helium at \(B = 10^8\) T as a function of the photon energy for linear polarisation obtained by summing over all initial states with \(|m| \leq 200\) and \(\nu \leq 2\) and assuming thermal occupation of the initial states. The cross section without thermal occupation from Fig. 4 is shown for comparison.

This effect becomes even more pronounced when we proceed to heavier elements such as oxygen (see Fig. 6). Below 100 eV practically no transitions contribute, and the peak around 100 eV becomes suppressed. The reason is that the energy difference between excited states and the ground state of oxygen is much larger than for helium, therefore the occupation probability is very small. In fact, we can show that there are only 600 transitions left which contribute significantly to the cross section. All
other transitions are negligible.

In the following, we concentrate on the total cross section for thermal occupation of the initial states with \( kT = 150 \text{ eV} \). Circularly polarised light is not considered in particular since it shows the same qualitative behavior as linearly polarised light.

### B. Photon density

We now take into account the temperature dependent spectral distribution of photons in the neutron star atmosphere, which we assume to be blackbody, and calculate total cross sections averaged over the photon energy distribution. It is these cross sections which are needed for the astrophysical modelling of the spectra of thermally emitting magnetised neutron stars. The starting point is Planck’s law divided by the photon frequency and, due to the assumption of a photon flux with one photon per volume element, normalized by the factor

\[
\int_0^\infty \tilde{P}(\omega, T) d\omega = \frac{4\pi T^3}{\alpha^2} 2\zeta(3),
\]

where \( \zeta(x) \) is the Riemann zeta function. This yields the photon density

\[
P(\omega, T) d\omega = \frac{\omega^2}{2\zeta(3) T^3} \frac{1}{e^{\omega/T} - 1} d\omega.
\]

The resulting photon density is shown in Fig. 4 for the temperature of \( kT = 150 \text{ eV} \).

The effect of the photon density is best shown in a comparison between the cross sections without photon density and the same cross section multiplied by the photon density \( P(\omega) \) (Fig. 7). The cross section changes its qualitative behavior towards the shape of the photon density. The peaks at energies around 20 eV are suppressed and the decay at energies greater than 400 eV is more rapid due to the low photon density.

The same picture for helium-like oxygen shows intriguing behavior (Fig. 8). The last two peaks around 2 keV originally have about the same value. When the photon density is taken into account the last peak is two orders of magnitude smaller. Thus the photon density can change the the shape of the final total cross section significantly.

### C. Density of the plasma

The atmosphere of a neutron star consists of ionised atoms. The volume an atom can fill is restricted by the particle density. Because of the enormous gravity at the surface neutron star atmospheres are strongly suppressed, and values for the mass density one finds in the literature range between \( \rho_p = 1 \text{ g/cm}^3 \) and \( \rho_p = 100 \text{ g/cm}^3 \) (see e.g. [11, 12]). Assuming that all atoms occupy the same state, the average volume available per atom \( V_n \) can be written as \( V_n = m_{\text{atom}}/\rho_p \) where \( m_{\text{atom}} \) is the atomic mass. No overlap of adjacent atoms with volumes smaller than \( V_n \) exists, and we have included only the contributions from these atomic states. We now wish to estimate for which mass densities in our calculations the restriction to \( |m| \leq 200 \) and \( \nu \leq 2 \) is justified, and whether or not for higher mass densities the maximum \( |m| \) can even be decreased.

We make the simple approximation that the atoms are cylindrically shaped and aligned gaplessly. As already noted the spatial extension \( \rho_\perp \) of a state perpendicular to the magnetic field is given by (7). We only consider the electron orbital with the largest extent, that is, with the maximum \( |m| \). The corresponding volume of the atom

![FIG. 6. (Color online) As Fig. 5 but for helium-like oxygen.](image-url)

![FIG. 7. (Color online) Total cross section for the photoionisation of helium at \( B = 10^8 \text{ T} \) obtained by summing over all initial states with \( |m| \leq 200 \) and \( \nu \leq 2 \) for thermal occupation of the initial states with \( kT = 150 \text{ eV} \), and averaged over a blackbody spectrum of the incident photon (linear polarisation) with the same temperature (lower dotted curve). The spectrally not averaged cross section from Fig. 5 (upper curve) is shown for comparison.](image-url)
FIG. 8. (Color online) As Fig. 7 but for helium-like oxygen at $B = 10^8$ T.

$\sigma_{\text{Th}}$ in $\text{g/cm}^3$ $\nu$ highest $|m|$ $N_i$

| $\rho$ in $\text{g/cm}^3$ | $\nu$ | $|m|$ | $N_i$ |
|----------------|------|------|-------|
| 0              | 0    | 199  |       |
| 1              | 1    | 169  | 336172|
| 2              | 2    | 125  |       |
| 10             | 0    | 36   |       |
| 1              | 1    | 22   | 4978  |
| 2              | 2    | 15   |       |
| 20             | 0    | 20   |       |
| 1              | 1    | 11   | 1400  |
| 2              | 2    | 7    |       |
| 50             | 0    | 9    | 282   |
| 1              | 1    | 4    |       |
| 2              | 2    | 2    |       |
| 100            | 0    | 5    |       |
| 1              | 1    | 2    | 71    |

TABLE I. Highest $|m|$ depending on $\nu$ at different plasma densities and the total number of transitions $N_i$.  

is $V_n = 2\pi\rho_0^2(|m|)$ \sqrt{\langle z^2 \rangle_{\text{max}}}$, where $\sqrt{\langle z^2 \rangle_{\text{max}}}$ denotes the maximum extension in z-direction. Generally, higher $\nu$ result in larger extensions. If the calculated volume $V_n$ is bigger than $V_s$, the state is omitted as an initial state. The same is true for final states.

In a more detailed treatment one would have to consider that the atoms are not purely cylindrical but cigar-shaped and therefore, more or less, aligned in an ellipsoidal packing. Moreover different states coexist, and the atoms are not aligned gaplessly but exhibit a separation. However, our simple approximation is good enough for the estimates that we are seeking For a more realistic approach, see e.g. [26].

In Table I we list, for five different mass densities the maximum $|m|$ depending on $\nu$ for which the volume of this state is still small enough to contribute to the cross section. This maximum quantum number declines fast for higher densities. It is interesting to note that some volumes of states with $\nu = 2$ at higher densities are still small enough. This is due to the very small $\rho_0$ if $m = 0$, and for two electrons the interaction with the nucleus is very strong so that $\langle z^2 \rangle$ increases only slowly. Therefore states with $m = 0$ can still be small enough, even if $\nu$ becomes very large. This also implies, that we still do not have a complete total cross section, but due to the low $|m|$ and $\nu$ seen in Table I it is possible to calculate all states and transitions in reasonable time.

The Table also shows that the number of transitions that have to be considered when calculating the total cross section. This number decreases rapidly, until at $100 \text{ g/cm}^3$ there is only 0.006% of the transitions necessary originally left.

Figure 9 shows the cross section, calculated for linearly polarised light, with mass densities between 1 and 100 g/cm$^3$. It can be seen that at 1 g/cm$^3$ the cross section changes only quantitatively, but not its qualitative behavior, while the number of transitions decreases by 740,000, which is 70% of the total transitions. The consequence is that many single cross section are negligible. Starting at 10 g/cm$^3$, the cross section is significantly changed. There is only a fraction of the originally calculated cross sections left, which is the reason for this huge change.

In particular, mostly highly excited states drop out. These transitions contribute to the lower energy range (1-50 eV) and this is why the cross section changes significantly in this range.

The reduction of the number and composition of tran-
sitions is important when calculating opacities. If oversized atoms are neglected, we know that no transitions are missing in the total cross section.

All physical conditions prevailing in the neutron star atmosphere are taken into account in Fig. 10 for a thermal occupation probability at $kT = 150$ eV, the photon density $P(\omega)$ with $kT = 150$ eV, and different plasma densities. The Figure shows that the peaks at energies between 10 and 50 eV are suppressed due to the low photon density, and the overall shift towards the shape of the photon density is obvious.

In all our calculations we have worked in the infinite-nuclear-mass approximation. We therefore finally discuss the influence of the finite nucleus mass on the results. It has been shown [1, 27] that the single-particle levels are raised by the cyclotron energy $\hbar \omega^+$ of the charged atomic nucleus. Intuitively this corresponds to its own gyration as a charged particle in the magnetic field. For the magnetic field strength considered here ($B = 10^8$ T), $\hbar \omega^+ = 1.67$ eV for helium, and 0.39 eV and 0.11 eV for helium-like oxygen and iron, respectively. This does not influence transition energies with $\Delta M = 0$, since all levels are raised by the same amount, and gives only a small correction for the, as compared to $\Delta M = 0$, weaker transitions with $\Delta M = \pm 1$.

VI. SUMMARY

We have developed a program code which allows calculating bound-free transitions of few-electron atoms and ions in neutron star magnetic fields in a routine way. For the examples of helium and helium-like oxygen we have analysed, for realistic physical parameters, which transitions contribute significantly to the total photoionisation cross sections and which are negligible. In this way we have succeeded in drastically reducing the numbers of transitions that have to be considered. The strategies developed in reducing the number of contributing transitions can also be applied in the calculation of the photoionisation of atoms and ions with more than two electrons.

The present results clearly demonstrate the complexity of ab-initio calculations of realistic photoionisation cross sections in neutron star magnetic fields that can be used in astrophysical modeling. An alternative would be the development of phenomenological models for the cross sections. Here our results could serve as useful starting point for developing such models.

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