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Analytic approximations to photoabsorption cross sections of once-ionized helium in magnetar atmospheres

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Abstract. Magnetar atmospheres can contain a substantial fraction of once-ionized helium. At the magnetic fields about 10^{14}–10^{15} G, typical of magnetars, Landau quantization is important not only for the electrons, but also for the centre-of-mass (CM) motion of the He$^+$ ion. The CM and internal motions are mutually dependent, which complicates theoretical studies of the He$^+$ characteristics. We present asymptotic analytic expressions for the binding energies, oscillator strengths, and photoionization cross sections of the moving hydrogenlike ions in an ultra-strong magnetic field, which can be used to construct approximate models of magnetar atmospheres.

1. Introduction

Magnetars are neutron stars with magnetic fields about 10^{14}–10^{15} G and effective temperatures up to $\sim 5 \times 10^6$ K (see, e.g., review [1]). Diffusive nuclear burning of hydrogen in magnetar envelopes can produce an atmosphere composed of helium [2]. At typical expected conditions in magnetar atmospheres, a large fraction of helium atoms can be once-ionized, while the high temperatures cause centre-of-mass (CM) motion of the helium ions across the magnetic field, affecting the properties of these ions and increasing their abundance [3].

Atomic and molecular systems in strong magnetic fields have been studied for several decades (see, e.g., extensive reviews [4, 5, 6]). The majority of the studies assumed the atomic nuclei to be infinitely massive (fixed in space). This assumption can serve as a convenient first approximation, but it is a gross simplification for astrophysical simulations, because thermal motion of atoms and ions across magnetic field lines breaks the cylindrical symmetry.

In strong magnetic fields of neutron stars, Landau quantization of the motion of the electrons and ions is important. The Coulomb interaction entangles the electron and ion motions, while the quantizing magnetic field hampers separation of the relative motions from the CM motion. The CM motion of an atom is characterized by its pseudomomentum. For an atomic ion, the two components of the pseudomomentum across the magnetic field do not commute, which complicates the problem still further.

Quantum-mechanical calculations of the characteristics of an one-electron ion (e.g., He$^+$) moving in a strong magnetic field were performed in [7, 8, 9], based on the formalism suggested in [10]. Following this approach, we derive practical expressions for the numerical treatment

of He$^+$ and other hydrogenlike ions moving in strong quantizing magnetic fields, which extend and supplement the previous results. In superstrong magnetic fields, we simplify the treatment using the adiabatic approximation. Furthermore, extending the method developed in [11] for a hydrogen atom to the hydrogenlike ions, we derive analytic formulae for quick evaluation of the binding energies, oscillator strengths, geometric sizes, and photoionization cross sections of such ions, which become exact in the limit of an ultra-strong magnetic field. The detailed mathematical derivation of the presented results is given in our preprint [12].

2. Basic formalism

2.1. One-electron ion in uniform magnetic field

Motion of two particles with masses m_- and m_+ and charges $-e$ and Ze in a magnetic field $\boldsymbol{B}$ directed along the z-axis is governed by the Hamiltonian

$$H_0 = \frac{1}{2m_-}\left(\boldsymbol{p}_- + \frac{e}{2c}\boldsymbol{B}\times\boldsymbol{r}_-\right)^2 + \frac{1}{2m_+}\left(\boldsymbol{p}_+ - \frac{Ze}{2c}\boldsymbol{B}\times\boldsymbol{r}_+\right)^2 - \frac{Ze^2}{|\boldsymbol{r}_- - \boldsymbol{r}_+|}, \qquad (1)$$

where $\boldsymbol{r}_\mp$ are the coordinate vectors and $\boldsymbol{p}_\mp$ are the respective canonical momenta. Here and hereafter we use the cylindrical gauge of the vector potential. The first two terms in Eq. (1) govern the free motion of the two particles in the field $\boldsymbol{B}$. The corresponding eigenstates are described by the Landau functions $\mathcal{F}_{n_-,\tilde{n}_-}^{(-1)}(\boldsymbol{r}_{-,\perp})$ and $\mathcal{F}_{n_+,\tilde{n}_+}^{(Z)}(\boldsymbol{r}_{+,\perp})$, defined by

$$\mathcal{F}_{n,\tilde{n}}^{(Z)}(\boldsymbol{r}_\perp) \equiv \frac{\mathrm{e}^{\mathrm{i}(\mathrm{sign}\,Z)(\tilde{n}-n)\varphi}}{\sqrt{2\pi/|Z|}\,a_{\mathrm{m}}}\,I_{\tilde{n},n}\left(\frac{|Z|r_\perp^2}{2a_{\mathrm{m}}^2}\right), \qquad (2)$$

where $a_{\mathrm{m}} = \sqrt{\hbar c/eB}$ is the magnetic length, $\boldsymbol{r}_\perp$ is the transverse component of the radius vector $\boldsymbol{r}$ and is defined by the polar coordinates $(r_\perp, \varphi)$, and $I_{\tilde{n},n}(x)$ is the Laguerre polynomial (see, e.g., [13]). The integer quantum numbers $n \geq 0$ and $\tilde{n} \geq 0$ are related, respectively, to the Landau energy level and to the square of the guiding centre $\boldsymbol{r}_c = (c/ZeB^2)\boldsymbol{k}\times\boldsymbol{B}$, where $\boldsymbol{k} = \boldsymbol{p} + (Ze/2c)\boldsymbol{B}\times\boldsymbol{r}$ is the pseudomomentum of the particle with charge Ze. The kinetic energy $E^\perp$ of the transverse motion of the two particles is independent of $\tilde{n}_\pm$,

$$E_{n_-,n_+}^\perp = \hbar\omega_{\mathrm{c}+}\left(n_+ + \frac{1}{2}\right) + \hbar\omega_{\mathrm{c}-}\left(n_- + \frac{1}{2}\right), \qquad (3)$$

where $\omega_{\mathrm{c}-} = eB/m_-c$ and $\omega_{\mathrm{c}+} = |Z|eB/m_+c$ are the respective cyclotron frequencies.

The principal difference between an atom and an atomic ion in a magnetic field appears clearly in the detailed mathematical study by Avron et al. [14]. For a neutral system, one can perform so called pseudoseparation of the collective motion, after which the resulting Hamiltonian for the internal degrees of freedom depends on the eigenvalues of the collective pseudomomentum. For a charged system, the number of integrals of motion is less than the number of degrees of freedom, therefore the collective and individual coordinates and momenta cannot be separated. Accordingly, the choice of good quantum numbers for a description of the considered system is a non-trivial problem. For a hydrogenlike ion, this problem was studied in detail in Ref. [10].

2.2. Expansion on the transverse basis

A convenient set of four quantum numbers related to the transverse motion of the two particles are the numbers $n_- \geq 0$ and $n_+ \geq 0$ related to the Landau excitations of the electron and the nucleus, the number L, which is the z-projection of the total angular momentum in units of $\hbar$, and the non-negative integer $\tilde{N}$ that enumerates eigenvalues of $K_\perp^2$, where $\boldsymbol{K}_\perp = \boldsymbol{k}_{-,\perp} + \boldsymbol{k}_{+\perp}$ is the transverse component of the total pseudomomentum. The numbers $\tilde{N}$ and L are more

convenient than $\tilde{n}_\pm$, because their generating operators commute with the Coulomb potential in Eq. (1). Moreover, $\tilde{N}$ and L enter the Schrödinger equation only in combination $\tilde{N} - L$.

Unlike $\tilde{N}$ and L, the Landau numbers n_- and n_+ are not conserved in the Coulomb potential. In general, a wave function ψ_κ of the two particles can be written as the superposition

$$\psi_\kappa(\boldsymbol{r}_{+,\perp}, \boldsymbol{r}_{-,\perp}, z) = \sum_{n_-, n_+} \Psi_{\tilde{N}, L, n_-, n_+}(\boldsymbol{r}_{+,\perp}, \boldsymbol{r}_{-,\perp})\, g_{n_- n_+; \kappa}(z), \tag{4}$$

where $\Psi_{\tilde{N}, L, n_-, n_+}(\boldsymbol{r}_{+,\perp}, \boldsymbol{r}_{-,\perp})$ describe the transverse motion of two non-interacting particles in the magnetic field, $z = z_- - z_+$ is the relative coordinate along the field and κ is a compound quantum number, which is assigned to the considered quantum state with energy E_κ and includes $\tilde{N}$ and L. The transverse basis in Eq. (4) can be written as [10]

$$\Psi_{\tilde{N}, L, n_-, n_+}(\boldsymbol{r}_{+,\perp}, \boldsymbol{r}_{-,\perp}) = U^\dagger \sum_{\tilde{n}=0}^{\mathcal{N}} (-1)^{n_- - \tilde{n}} C_{\tilde{n}}^{(\mathcal{N}, n_+)} \mathcal{F}_{\mathcal{N}-\tilde{n}, \tilde{N}}^{(Z-1)}(\boldsymbol{r}_{+,\perp}) \mathcal{F}_{\tilde{n}, n_-}^{(1)}(\boldsymbol{r}_\perp), \tag{5}$$

where $U^\dagger = \exp\left[-(\mathrm{i}e/2\hbar c)(\boldsymbol{B} \times \boldsymbol{r}_+) \cdot \boldsymbol{r}_-\right]$ is the unitary transformation operator, $\mathcal{N} \equiv \tilde{N} - L + n_-$, and $n_+ = 0, 1, 2, \ldots, \mathcal{N}$. The coefficients $C_{\tilde{n}}^{(\mathcal{N}, n_+)}$ can be calculated using recurrence relations (see details in [12]).

In Eq. (4), $g_{n_- n_+; \kappa}(z)$ are the "longitudinal wave functions" to be determined. Substitution of Eq. (4) into the Schrödinger equation with the Hamiltonian (1) leads to the system of equations

$$\left(\frac{p_z^2}{2m_*} - E_\kappa^\parallel\right) g_{n_- n_+; \kappa}(z) = -\sum_{n'_-=0}^{\infty} \sum_{n'_+=0}^{\mathcal{N}} V_{n'_-, n'_+; n_-, n_+}^{(\tilde{N}-L)}(z)\, g_{n'_- n'_+; \kappa}(z), \tag{6}$$

where $E_\kappa^\parallel \equiv E_\kappa - E_{n_-, n_+}^\perp$, $m_* = m_+ m_-/(m_+ + m_-)$ is the reduced mass, $p_z = -\mathrm{i}\hbar\partial/\partial z$,

$$V_{n'_-, n'_+; n_-, n_+}^{(\tilde{N}-L)}(z) = \sum_{k=k_{\min}}^{\mathcal{N}} C_{n'_- - n_- + k}^{(\mathcal{N}', n'_+)} C_k^{(\mathcal{N}, n_+)} \int_{R^2} \mathcal{F}_{n'_-, n'_- - n_- + k}^{(-1)*}(\boldsymbol{r}_\perp) \frac{-Ze^2}{\sqrt{r_\perp^2 + z^2}} \mathcal{F}_{n_-, k}^{(-1)}(\boldsymbol{r}_\perp)\, \mathrm{d}^2 r_\perp, \tag{7}$$

is an effective one-dimensional potential, $\mathcal{N}' = \tilde{N} - L + n'_-$, $\mathcal{N} = \tilde{N} - L + n_-$, and $k_{\min} = \max(0, n_- - n'_-)$. The quantum states can be numbered as $|\kappa\rangle = |\tilde{N}, L, n_{0-}, n_{0+}, \nu\rangle$, where, n_{0-} and n_{0+} are the values of n_- and n_+ for the leading term in expansion (4), and ν relates to the "longitudinal" degrees of freedom; $\nu = 0, 1, 2, \ldots$ for the bound states and $\nu = (E, \pm)$ for the continuum, where E is the energy and $\pm$ the z-parity.

In the superstrong magnetic fields, potentials $V_{n'_-, n'_+; n_-, n_+}^{(\tilde{N}-L)}(z)$ with $n'_- \neq n_-$ or $n'_+ \neq n_+$ are relatively small on the typical z-scales of the functions $g_{n_- n_+; \kappa}(z)$, compared to the potentials with $n'_- = n_-$ and $n'_+ = n_+$. Keeping only the latter "diagonal" terms, one arrives at the *adiabatic approximation*, where the wave function ψ_κ is factorized into $\Psi_{\tilde{N}, L, n_-, n_+}(\boldsymbol{r}_{+,\perp}, \boldsymbol{r}_{-,\perp}) g_{n_- n_+; \kappa}(z)$. We will use this approximation to obtain analytic solutions. Since the electron cyclotron energy $\hbar\omega_{\mathrm{c}-} \sim (B/10^{14}\,\mathrm{G})$ MeV is huge in the magnetars, we set $n_- = 0$ and suppress the subscript n_- hereafter.

3. Bound states in the adiabatic approximation

In the adiabatic approximation, Eq. (6) reduces to the 1D Schrödinger equation with the effective potential $V_{n_+}^{(\tilde{N}-L)}(z)$ resembling the truncated one-dimensional (1D) Coulomb potential, analogous to the 1D H atom problem. It is well known (see, e.g., [15] and references therein)

that in this case the discrete energy spectrum contains a "tightly bound" level $\nu = 0$, whose binding energy increases logarithmically with increasing B, and levels $\nu = 1, 2, 3, \ldots$, whose binding energies resemble the field-free H series. The latter "H-like states" are expected to be weakly occupied in the magnetar atmospheres.

Calculations similar to [11] give the following equation (see [12] for details):

$$\pi \cot \tilde{\nu} \pi + \Theta(\tilde{\nu}) = \ln \frac{a_*}{2a_{\mathrm{m}}} + \frac{\ln 2 - 3\gamma_{\mathrm{E}} - J_{\mathcal{N}n_+}}{2} \tag{8}$$

$(|\sin \tilde{\nu} \pi| \ll 1)$, where $a_* = \hbar^2/m_* Z e^2$, $\Theta(\tilde{\nu})$ is defined by the expression

$$\Theta(\tilde{\nu}) = \ln \tilde{\nu} - \frac{1}{2\tilde{\nu}} - \psi(\tilde{\nu}) = \ln \tilde{\nu} + \frac{1}{2\tilde{\nu}} - \psi(1 + \tilde{\nu}), \tag{9}$$

$\psi(x)$ is the digamma function, $\tilde{\nu}$ is the "effective principal quantum number" defined by relation $\epsilon_\kappa \equiv |E_\kappa^\parallel|/\mathrm{Ry}_* \equiv \tilde{\nu}^{-2}$, and $\mathrm{Ry}_* \equiv Z^2 e^4 m_*/2\hbar^2$ is the effective Rydberg energy: $\mathrm{Ry}_* = Z^2 (m_*/m_e)\mathrm{Ry}$, where $\mathrm{Ry} \equiv e^2/2a_{\mathrm{B}}$, $a_{\mathrm{B}} = \hbar^2/m_e e^2$ is the Bohr radius and m_e is the electron mass. The novel term

$$J_{\mathcal{N}n_+} = \sum_{k=1}^{\mathcal{N}} \sum_{n=1}^{k} \frac{1}{n} \left(C_k^{(\mathcal{N},n_+)} \right)^2 \quad (\mathcal{N} \geq 1, \ 0 \leq n_+ \leq \mathcal{N}) \tag{10}$$

arises due to the CM motion of the ion. For a non-moving ion $\mathcal{N} = 0$, $J_{00} = 0$, and the known result [11] is recovered. Solution of Eq. (8) gives the longitudinal energies $E_\kappa^\parallel$.

The tightly bound states correspond to $\tilde{\nu} \ll 1$. In this case, we get approximately

$$\frac{1}{\tilde{\nu}} = \ln \frac{\gamma_*}{2} + 2 \ln \tilde{\nu} - \gamma_{\mathrm{E}} - J_{\mathcal{N}n_+} + \frac{\pi^2}{3} \tilde{\nu}, \tag{11}$$

where we have introduced the magnetic-field parameter $\gamma_* = \hbar^3 B/Z^2 m_*^2 e^3 c = B/B_*$, which should be large in the considered approximation. Here, $B_* \equiv Z^2 m_*^2 e^3 c/\hbar^3 \approx 2.35 \times 10^9 (m_*/m_e)^2 Z^2$ G.

In the adiabatic approximation one can prove [12] that the mean-squared transverse geometric sizes of the H-like ions $\langle \kappa | r_\perp^2 | \kappa \rangle$ linearly depend on the quantum numbers $\mathcal{N}$ and n_+. In the particular case of the He$^+$ ions ($Z = 2$) they become independent of n_+, $\langle \kappa | r_\perp^2 | \kappa \rangle = (2 + \mathcal{N})a_{\mathrm{m}}^2$.

4. Radiative transitions for circular polarization

4.1. Bound-bound transitions

In the dipole approximation, the cross section of bound-bound radiative transitions from state $|i\rangle = |\kappa\rangle$ to state $|f\rangle = |\kappa'\rangle$ can be written as

$$\sigma_{i \to f, \alpha}^{\mathrm{bb}}(\omega) = 2\pi^2 \frac{e^2}{m_e c} f_{fi,\alpha} \Delta_{fi}(\omega), \tag{12}$$

where

$$f_{fi,\alpha} = \frac{\hbar \omega}{\mathrm{Ry}} \left| \frac{D_{fi,-\alpha}}{e a_{\mathrm{B}}} \right|^2 \tag{13}$$

is the oscillator strength, which is defined following [11], α is the photon polarization index, corresponding to the cyclic components of the polarization vector $\boldsymbol{e}$, so that $e_{\pm 1} \equiv (e_x \pm e_y)/\sqrt{2}$, $\Delta_{fi}(\omega - \omega_{fi})$ describes the profile of the spectral line at photon energies $\hbar\omega$ around $\hbar\omega_{fi} = E_f - E_i$, normalized so that $\int \Delta_{fi}(\omega)\, \mathrm{d}\omega = 1$, and $D_{fi,-\alpha}$ is the corresponding cyclic component

of the electric dipole matrix element. The conservation of the total angular momentum requires $L_f = L_i + \alpha$. In the adiabatic approximation, the dipole matrix element for the radiative transitions from state $|i\rangle = |\kappa\rangle$ to state $|f\rangle = |\kappa'\rangle$ with $n_- = n'_- = 0$ reduces to

$$D_{fi,-\alpha} = e a_{\mathrm{m}} \sqrt{Z\, n_+^{\max}}\, \mathcal{L}(\kappa'|\kappa)\, \delta_{n'_+, n_+ + \alpha} \delta_{\mathcal{N}', \mathcal{N} + \alpha}, \qquad (14)$$

where $n'_+ = n_+ + \alpha$, $n_+^{\max} = \max(n_+, n'_+)$, and $\mathcal{L}(\kappa'|\kappa) \equiv \int g_{\kappa'}^*(z) g_\kappa(z)\, \mathrm{d}z$ is the overlap integral, both g_κ and $g_{\kappa'}$ being normalized to 1 in the integration range. Using the technique similar to [11], we obtained [12] analytic asymptotic expressions for $|\mathcal{L}(\kappa'|\kappa)|$. In the particular case of the tightly bound states,

$$\mathcal{L}^2(\kappa'|\kappa) \approx \left(1 + \frac{2}{\ln(\gamma_*/2)}\right)^{-2} \sim 1 - \frac{4}{\ln \gamma_*}. \qquad (15)$$

Thus for the transitions between tightly-bound states we obtain the following approximate expression for the oscillator strength to the leading order in $1/\ln \gamma_*$:

$$f_{fi,\alpha} = \frac{\hbar \omega}{\mathrm{Ry}} \frac{a_{\mathrm{m}}^2}{a_{\mathrm{B}}^2} Z\, n_+^{\max} \left(1 - \frac{4}{\ln \gamma_*}\right) \delta_{n'_+, n_+ + \alpha} \delta_{\mathcal{N}', \mathcal{N} + \alpha}. \qquad (16)$$

4.2. Photoionization

For the bound-free transitions, using once again the adiabatic and dipole approximations and applying the technique similar to [11], we obtain the following asymptotic expression for the cross section:

$$\sigma_{i \to f, \alpha}^{\mathrm{bf}}(\omega) = \frac{4e^2}{\hbar c}\, n_+^{\max} a_{\mathrm{m}}^2 \frac{\hbar \omega}{\mathrm{Ry}_*} \left[1 - \exp\left(-\frac{2\pi}{\sqrt{\epsilon_f}}\right)\right] S_f\, \sqrt{\epsilon_i} \left(\frac{J_{\mathcal{N}'n'_+} - J_{\mathcal{N}n_+}}{\epsilon_f + \epsilon_i}\right)^2 \delta_{n'_+, n_+ + \alpha}\, \delta_{\mathcal{N}', \mathcal{N} + \alpha}, \qquad (17)$$

where

$$S_f = \left\{1 + \left(\frac{1 - \mathrm{e}^{-2\pi\tilde{\nu}'}}{2\pi}\right)^2 \left[\ln \frac{\gamma_*}{2} - 3\gamma_{\mathrm{E}} + J_{\mathcal{N}'n'_+} + 2\ln \tilde{\nu}' - 2\,\mathrm{Re}\,\psi(1 + \mathrm{i}\tilde{\nu}')\right]^2\right\}^{-1}. \qquad (18)$$

It generalizes an analogous expression for the photoionization of the H atom in a strong magnetic field, derived in [16], to the case of a H-like ion (see [12] for the mathematical derivation and for an efficient calculation algorithm).

Examples of the photoionization cross sections of He$^+$ in this approximation are shown in Fig. 1 for $B = 10^{14}$ G and 5×10^{14} G. In the latter case, results are shown only for $n_+ = 0$ and $n_+ = 1$, because the states with $n_+ \geq 2$ belong to the continuum (i.e., have $E_i > 0$), since $2\hbar\omega_{\mathrm{c}+} > |E_\kappa^{\parallel}|$ at such strong field. This means that these states should be autoionizing through the coupled channels in Eq. (6) beyond the adiabatic approximation. The cross sections in Fig. 1 are defined for $\hbar\omega > \hbar\omega_{\mathrm{thr}} = -E_i = |E_i^{\parallel}| + \alpha\hbar\omega_{\mathrm{c}+}$, where the longitudinal energies $E_i^{\parallel}$ are calculated according to the approximation (11). The cross sections decrease with increasing B. They also become smaller with increasing $\mathcal{N}$ at fixed n_+ and ω.

5. Conclusions

We performed an approximate analytic treatment of the photoabsorption of once-ionized helium in ultra-strong magnetic fields in the adiabatic approximation and derived explicit asymptotic expressions for the binding energies, transverse geometric sizes, and cross sections of absorption of radiation, polarized transversely to the magnetic field. We expect that these expressions can be useful in the case of superstrong magnetic fields, typical for magnetars.
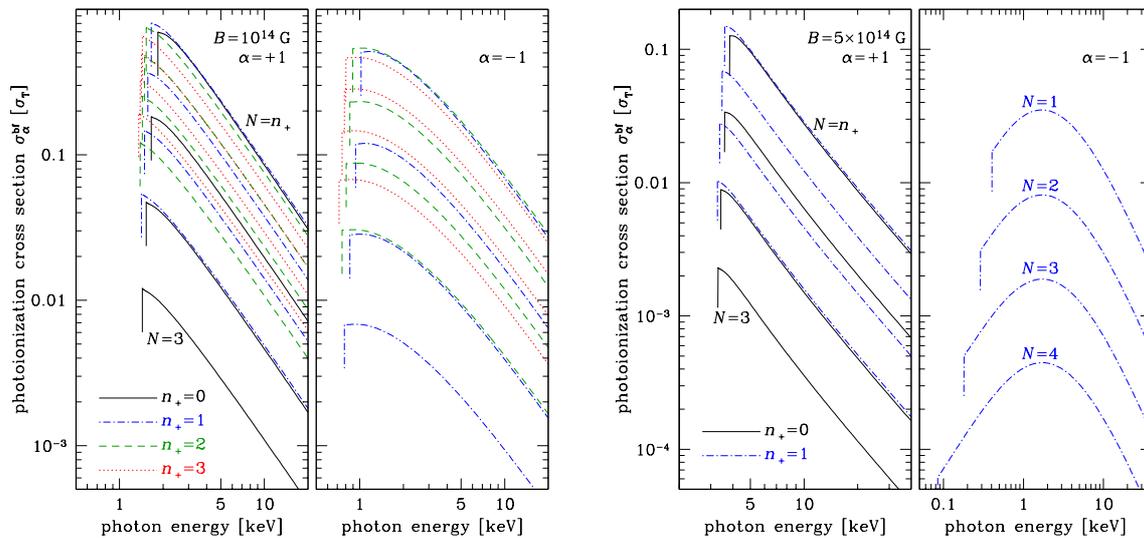
Figure 1. Photoionization cross sections $\sigma_{i \to f, \alpha}^{\mathrm{bf}}(\omega)$ for different initial tightly-bound states $|i\rangle = |\mathcal{N}, n_-, n_+, \nu\rangle$ $(n_- = 0,\ \nu = 0)$ at $B = 10^{14}$ G (two left panels) and 5×10^{14} G (two right panels) in the adiabatic approximation according to Eq. (17) for the right $(\alpha = +1)$ and left $(\alpha = -1)$ circular polarizations as functions of the photon energy $\hbar\omega$ in units of Thomson cross section. The results in the left panels are displayed for initial states with quantum numbers $n_+ = 0$ (solid lines), 1 (dot-dashed lines), 2 (dashed lines), and 3 (dotted lines) and $\mathcal{N} = n_+, n_+ + 1, n_+ + 2, n_+ + 3$ (lines of the same type from top to bottom for each n_+; only the cases of $n_+ = 0$ and $n_+ = 1$ are shown in the right panels).

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