One-electron ion in a quantizing magnetic field

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A charged particle in a magnetic field possesses discrete energy levels associated with particle rotation around the field lines. A bound complex of particles with a nonzero net charge possesses analogous levels associated with its center-of-mass motion and, in addition, the levels associated with internal degrees of freedom, that is with relative motions of its constituent particles. The center-of-mass and internal motions are mutually dependent, which complicates theoretical studies of the binding energies, radiative transitions and other properties of the complex ions moving in quantizing magnetic fields. In this work, we present a detailed derivation of practical expressions for the numerical treatment of such properties of the hydrogen-like ions moving in strong quantizing magnetic fields, which follows and supplements the previous works of Bezchastnov et al. Second, we derive asymptotic analytic expressions for the binding energies, oscillator strengths, and photoionization cross sections of the moving hydrogen-like ions in the limit of an ultra-strong magnetic field.

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Contents

I. Introduction
II. Generalities
A. Charged particle in uniform magnetic field
B. Two charged particles in uniform magnetic field
III. Transverse basis
A. Canonical transformations
B. Creation and annihilation operators
C. Good quantum numbers
D. Transverse basis states
E. Recurrence relations for the basis coefficients
IV. Solution of the Schrödinger equation
A. Expansion on the transverse basis
B. Calculation of effective potentials
C. Adiabatic approximation
D. Coupled channel formalism
1. Bound-state wave functions
2. Continuum wave functions
E. Geometric sizes of the ions
V. Interaction with radiation
A. Radiative transitions
B. Dipole approximation
C. Expansion on the transverse basis
VI. Approximate solutions for ultra-strong fields
A. Wave functions and eigenenergies
1. Exterior solution for bound states
2. Interior solution for even states
3. Binding energies of even states
4. Odd bound states
5. Continuum states
B. Overlap integrals between even states
1. The case of tightly bound states
2. Overlaps of tightly bound states with other even states
3. The bound-free case
C. Transverse geometric size
D. Radiative transitions for circular polarization
VII. Conclusions
Acknowledgments
Appendices
A. Supplementary relations for $C_k^{(N,n_+)}$
B. Proof of Equation (202)
C. Estimate of $J_{N_0}$ at large $N$
D. Calculation of $\text{Re} \Theta(i\tilde{\nu})$
E. Proof of Equation (249)
References

I. INTRODUCTION

Properties of atomic and molecular systems in external magnetic fields have been intensively studied for several decades (see, e.g., extensive reviews [2–4]). The majority of the studies considered them to be at rest and assumed the atomic nuclei to be infinitely massive (fixed in space). The model of infinitely massive nuclei can serve as a convenient first approximation, but it is a gross simplifica-
tion for astrophysical simulations, because thermal motion of atoms and ions across magnetic field lines breaks the axial symmetry.

The theory of motion of a system of point charges in a constant magnetic field is reviewed in [2, 3]. A comprehensive calculation of hydrogen-atom energy spectra, taking account of the effects of motion across the strong magnetic fields, was carried out in Refs. [4, 5]. Calculations of the rates of different types of radiative transitions and the absorption coefficients in neutron star atmospheres were performed in a series of studies (e.g., Refs. [6, 7], and references therein). Based on these data, a model of the hydrogen atmosphere of a neutron star with a strong magnetic field was elaborated [11]. The database for astrophysical calculations was created using this model in Refs. [12, 13] (see also the review [14]).

In Sect. II we present the general formalism for treating one and two charged particles in a uniform magnetic field and introduce basic notations. In Sect. III we present a detailed derivation of the convenient basis of orbitals [18] for treating the problem of two charged particles in a strong magnetic field (as a by-product, we notice some corrections to Ref. [18] near the end of Sect. III). Section IV is devoted to the solution of the Schrödinger equation for astrophysical simulations, because thermal motion across the strong magnetic field were performed in Refs. [15–17], and references therein). Based on these data, a model of the hydrogen atmosphere of a neutron star with a strong magnetic field was elaborated [11]. The database for astrophysical calculations was created using this model in Refs. [12, 13] (see also the review [14]).

In Sect. II we present the general formalism for treating one and two charged particles in a uniform magnetic field and introduce basic notations. In Sect. III we present a detailed derivation of the convenient basis of orbitals [18] for treating the problem of two charged particles in a strong magnetic field (as a by-product, we notice some corrections to Ref. [18] near the end of Sect. III). Section IV is devoted to the solution of the Schrödinger equation and calculation of the main properties of the two-particle system using the basis constructed in Sect. III. In Sect. V we present general formulas for treating interaction of such system of particles with radiation, based on the solution described in Sect. IV. In Sect. VI following and extending the method of Hasegawa & Howard [19] and using the theory described in the preceding sections, we derive analytic approximations for wave functions, binding energies, the transverse geometric size, overlap integrals and oscillator strengths between different quantum states, and photoionization cross sections of a one-electron ion. Section VII presents the conclusions. In Appendices we derive some useful supplementary relations and prove some statements from the main text.

II. GENERALITIES

A. Charged particle in uniform magnetic field

The quantum-mechanical problem of motion of a charged particle in a uniform and constant magnetic field was first solved by Rabi [20] and Landau [21]. In this subsection we expose this solution for completeness and introduce some basic notations.

Let us consider a motion of a free particle with a positive or negative charge $Ze$, where $e$ is the elementary charge, in a uniform magnetic field $B$. The Hamiltonian equals the kinetic energy operator

$$H^{(1)} = \frac{m\dot{r}^2}{2} = H^{(1)}_\perp + \frac{p_z^2}{2m}, \quad H^{(1)}_\perp = \frac{\pi^2}{2m},$$

where $m$ is the mass,

$$\pi = m\dot{r} = p - \frac{Ze}{c} A(r)$$

is the kinetic momentum, $A(r)$ is the vector potential of the field, and $p = -i\hbar \nabla$ is the canonical momentum operator conjugate to $r$. In Eq. (1) and hereafter, “$\perp$” denotes the “transverse” part, related to the motion in the $xy$ plane, while $B$ is along the $z$-axis.

A classical particle moves along a spiral around the normal to the $xy$ plane at the guiding center $r_c$. In quantum mechanics, $r_c$ is an operator, related to the pseudomomentum operator $k$:

$$k = m\dot{r} + \frac{Ze}{c} B \times r = p - \frac{Ze}{c} A(r) + \frac{Ze}{c} B \times r,$$

$$r_c = \frac{c}{ZeB^2} k \times B.$$  (3)

The pseudomomentum is a constant of motion in a homogeneous magnetic field (unlike the canonical momentum and the kinetic momentum, which are not conserved). Coordinate operators of $r_c$ commute with $H^{(1)}_\perp$, but do not commute with each other: $[x_c, y_c] = -i\hbar c/(ZeB)$.

Another constant of motion, which generalizes the parallel component of the orbital momentum $l$, is

$$l_z = \hat{z} \cdot (r \times \frac{k + \pi}{2}) = \frac{c}{2ZeB} (k^2 - \pi^2),$$

where $\hat{z} = B/B$ is the unit vector in the magnetic field direction.

In general, $H^{(1)}_\perp$ should be supplemented by $(-B \cdot \hat{\mu})$, where $\hat{\mu} = g_{m_{\text{mag}}} (e/2mc) \hat{S}$ is the intrinsic magnetic moment of the particle, $\hat{S}$ is the spin operator, and $g_{m_{\text{mag}}}$ is the spin $g$-factor ($g_{m_{\text{mag}}} = -2.0023$ and 5.5857 for the electron and the proton, respectively). We do not consider the spin term at the moment.

Quantum states with definite eigenvalue $\hbar k_z$ of the longitudinal momentum $p_z$ in $H^{(1)}$ are described by the wave functions

$$\psi(r) = C_{\text{norm}} e^{ik_z z} \Phi^{(2)}(r_\perp),$$

where $k$ and $\Phi^{(2)}(r_\perp)$ in $r_\perp$ are the wave number and the radial part of the wave function in the transverse plane, respectively.
where $C_{\text{norm}}$ is a normalization constant and $r_\perp = (x,y) = (r_\perp \cos \varphi, r_\perp \sin \varphi)$. The form of the function $\Phi^Z(r_\perp)$ depends on a choice of the gauge for $A(r)$. Let us consider the cylindrical gauge

$$A = \frac{1}{2} B \times r.$$  

Then $\nabla \cdot A = 0$, $A^2 = B^2 r_\perp^2$, and $A \cdot p = p \cdot A = \frac{1}{2} (B \times r) \cdot p$. Therefore,

$$(p \cdot A + A \cdot p) \psi = -i \hbar \left[ \nabla \cdot (A \psi) + A \cdot \nabla \psi \right]
= -i \hbar (\psi \nabla \cdot A + 2 A \cdot \nabla \psi)
= 2 A \cdot p \psi,$$  

so that

$$\pi^2 = \left( p - \frac{Ze}{c} A \right)^2
= p^2 - \frac{Ze}{c} (p \cdot A + A \cdot p) + \left( \frac{Ze}{c} \right)^2 A^2
= p^2 - \frac{Ze}{c} B l_z + \left( \frac{Ze}{2c} \right)^2 B^2 r_\perp^2,$$  

where $l_z$ is defined by Eq. (25). In the cylindrical gauge $(k + \pi)/2 = p$, therefore $l_z$ takes the same form as without the field.

For $H_\perp^{(1)}$ we have the following eigenvalue problem:

$$\left( \frac{p^2}{2m} - \frac{\sigma \omega_c}{2} l_z + \frac{m \omega_c^2 r_\perp^2}{8} \right) \Phi = E_\perp \Phi,$$  

where $\omega_c = |Z| eB/mc$ is the cyclotron frequency and $\sigma \equiv \text{sign} Z$. Since $l_z$ is an integral of motion, a solution to Eq. (10) can be found separately for each its eigenvalue $\lambda$ with integer $n$, such that it can be written in the polar coordinate system $(r_\perp, \varphi)$, in the $(x,y)$ plane as

$$\Phi^Z(r_\perp, \varphi) = f(r_\perp) \frac{e^{i \lambda \varphi}}{\sqrt{2 \pi}}.$$  

Substitution of function (11) into Eq. (10) gives

$$-\frac{h^2}{2m} \frac{1}{r_\perp} \frac{d}{dr_\perp} \left( r_\perp \frac{df}{dr_\perp} \right) + \left( \frac{\hbar^2 \lambda^2}{2m r_\perp^2} + \frac{m \omega_c^2 r_\perp^2}{8} \right) f
= \left( E_\perp + \sigma \frac{\hbar \omega_c}{2} \lambda \right) f.$$  

Let us introduce notations

$$\rho = \frac{r_\perp^2}{2a_{m,z}}, \quad \kappa = \frac{E_\perp}{\hbar \omega_c} + \sigma \frac{\lambda}{2},$$  

where

$$a_{m,z} = \sqrt{\frac{\hbar}{m \omega_c}} = \frac{a_m}{\sqrt{|Z|}}$$  

and $a_m = \sqrt{\hbar e/B}$ is the magnetic length. Then Eq. (12) becomes

$$\frac{d^2 f}{d\rho^2} + \frac{1}{\rho} \frac{df}{d\rho} + \kappa \frac{\lambda^2}{4 \rho^2} f = 0.$$  

At $\rho \to 0$, it turns into the Cauchy-Euler equation

$$\frac{d^2 f}{d\rho^2} + \frac{1}{\rho} \frac{df}{d\rho} - \frac{\lambda^2}{4 \rho^2} f = 0,$$  

which has the explicit solution $f = A_1 \rho^{\lambda/2} + A_2 \rho^{-\lambda/2}$. Normalizability of $\psi(r_\perp, \varphi)$ requires that we select a solution with non-negative power, $f \sim \rho^{\lambda/2} \sim r_\perp^{\lambda/2}$ at $\rho \to 0$. Substitution of $f = \rho^{\lambda/2} e^{-\rho^2/2}$ gives the confluent hypergeometric equation

$$\rho^2 \frac{d^2 y}{d\rho^2} + (|\lambda| + 1 - \rho) \frac{dy}{d\rho} - \frac{|\lambda| + 1}{2} + \kappa = 0,$$  

Its solution is the Kummer function \[22\], which provides a finite $f$ at $\rho \to \infty$ only under the condition that

$$\kappa - \frac{|\lambda| + 1}{2} = n_r,$$  

where $n_r$ is non-negative integer, called radial quantum number. Recalling Eq. (13), we obtain

$$E_\perp = \hbar \omega_c \left( n_r + \frac{1}{2} + \frac{|\lambda| - \sigma \lambda}{2} \right)$$  

and

$$y(\rho) = CL_\nu^{\lambda}(\rho),$$  

where $L_\nu^{\lambda}(\rho)$ is a generalized Laguerre polynomial \[22\] and $C$ is a normalization constant. Therefore, the normalized solutions to Eq. (10) can be written as

$$\Phi_{n,s}^{(Z)}(r_\perp) = \frac{\exp(|\lambda| \varphi)}{\sqrt{2 \pi} a_{m,z}} I_{n+s,n} \left( \frac{r_\perp^2}{2a_{m,z}^2} \right),$$  

and

$$E_{\perp,n}^{(Z)} = \hbar \omega_c \left( n + \frac{1}{2} \right),$$  

where

$$s = \sigma \lambda, \quad n = n_r + \frac{|\lambda| - s}{2}$$  

and $I_{n,s}(\rho) (n' = n + s)$ are the normalized Laguerre functions \[23\], which are proportional to $e^{-\rho^2/2} \rho^{n'-n}/2 L_{n'}^{n'}(\rho)$ and are normalized so that

$$\int_0^\infty I_{n,s}^2(\rho) d\rho = 1.$$  

Explicitly,
\[ I_{n',n}(\rho) = e^{-\rho/2}\rho^{(n'-n)/2}\sum_{k=0}^{n} (-1)^k \sqrt{n!} \rho^k \]
if \( n' \geq n \);
\[ I_{n',n}(\rho) = (-1)^{n'-n} I_{n,n'}(\rho), \quad \text{if } n' < n . \] (25a)

The number \( n \) in Eq. (23) enumerates the Landau energy levels (e.g., Ref. [24]). Its definition implies that, for a given Landau level, the quantum number \( s \) is bounded from below:
\[ s = -n,-n+1,-n+2, \ldots \] (26)

The functions \( \Phi_{n,s}^{(1)}(r_\perp) \), which describe electron motion perpendicular to magnetic field, are often called Landau functions. They satisfy the condition of orthogonality
\[ \int_{S^2} dr_\perp \Phi_{n,s}^{(1)}(r_\perp) \Phi_{n',s'}^{(1)}(r_\perp) = \delta_{n,n'}\delta_{s,s'} \] (27)
and completeness
\[ \sum_{n,s} \Phi_{n,s}^{(1)}(r_\perp) \Phi_{n,s}^{(1)}(r_\perp) = \delta(r_\perp - r_\perp) . \] (28)
Therefore they form a complete basis in a Hilbert space.

By construction, \( \Phi_{n,s}^{(1)}(r_\perp) \) is an eigenfunction of the orbital momentum projection operator \( l_z \), with eigenvalue \( \lambda = s \sigma \) and an eigenfunction of the squared transverse kinetic momentum operator \( \pi_\perp^2 = 2mH_\perp(1) \) with eigenvalue \( mh_\omega(2n+1) \). Therefore, according to Eq. (5), it is also an eigenfunction of the squared transverse pseudomomentum operator \( k^2 \) with eigenvalue \( mh_\omega(2n+1) \), where \( \hat{n} = n + \sigma = n + s \). We can identify the eigenstates using the pair of numbers \((n,\hat{n})\) instead of \((n,s)\) and accordingly to define the Landau functions with modified subscripts (e.g., [17][18]),
\[ F_{n,n}(r_\perp) = \Phi_{n,n}(r_\perp) = \frac{e^{i\sigma(n-n)\varphi}}{\sqrt{2\pi} a_m Z} I_{n,n} \left( \frac{r_\perp^2}{2a_m^2 Z} \right) \] (29)
whose \( \sigma = \text{sign } Z, a_m, Z \equiv a_m, \sqrt{Z} \). From Eq. (25a) we see that
\[ F_{n,n}(r_\perp) = (-1)^{\hat{n}-n} F_{n,n}(r_\perp) = F_{\hat{n},n}(-r_\perp) . \] (30)

Let us define cyclic components of any vector \( a \) as
\[ a_{\pm 1} = \frac{ax \pm iay}{\sqrt{2}}, \quad a_0 = a_z . \] (31)

The transverse cyclic components of the kinetic momentum operator and of the pseudomomentum operator transform one Landau state \( |n,\hat{n}\rangle \), characterized by \( F_{n,n}(r_\perp) \), into another Landau state:
\[ \pi_\alpha |n,\hat{n}\rangle_\perp = -i\sigma \alpha \frac{\hbar}{a_m} \sqrt{n + 1/2 - \sigma \alpha/2} n - \sigma \alpha, \hat{n} \rangle, \] (32)
\[ k_\alpha |n,\hat{n}\rangle_\perp = i\sigma \alpha \frac{\hbar}{a_m} \sqrt{n + 1/2 + \sigma \alpha/2} |n,\hat{n} + \sigma \alpha \rangle, \] (33)
where \( \alpha = \pm 1 \) and \( \sigma = \text{sign } Z \).

B. Two charged particles in uniform magnetic field

Motion of two particles with masses \( m_- \) and \( m_+ \) and charges \( -e \) and \( Ze \) \((e > 0, Z > 1)\) in a homogeneous magnetic field \( B = (0,0,B) \) is governed by the Hamiltonian
\[ H_0 = \frac{\pi_+^2}{2m_+} + \frac{\pi_-^2}{2m_-} + V_C = \frac{p_{\perp}^2}{2m_-} + \frac{p_{\perp}^2}{2m_+} + H_\perp + V_C, \] (34)
where
\[ H_\perp = \frac{\pi_+^2}{2m_-} + \frac{\pi_-^2}{2m_+} \] (35)
determines the motion of the two non-interacting particles according to Eq. (11),
\[ \pi_- = p_- + \frac{e}{2c} B \times r_-, \quad \pi_+ = p_+ - \frac{Ze}{2c} B \times r_+ \] (36)
are the kinetic momenta, and
\[ V_C = -\frac{Ze^2}{|r_- - r_+|} \] (37)
is the Coulomb potential.

Longitudinal motion of the system as a whole can be factorized out by introducing the \( z \)-coordinate of center-of-mass \( Z = (m_+ z_+ + m_- z_-)/M \), where \( M = m_+ + m_- \), and the relative coordinate \( z = z_+ - z_- \). The change of variables \((z_-, z_+) \rightarrow (z_{cm}, z)\) implies
\[ \frac{\partial}{\partial z_\pm} = \frac{\partial z_{cm}}{\partial z_\pm} \frac{\partial}{\partial z_{cm}} + \frac{\partial z}{\partial z_\pm} \frac{\partial}{\partial z} = \frac{m_\mp}{M} \frac{\partial}{\partial z_{cm}} \pm \frac{\partial}{\partial z}; \]
\[ \frac{\partial^2}{\partial z_\pm^2} = \left( \frac{m_\mp}{M} \right)^2 \frac{\partial^2}{\partial z_{cm}^2} \pm 2\frac{m_\mp}{M} \frac{\partial}{\partial z_{cm}} \frac{\partial}{\partial z} + \frac{\partial}{\partial z^2} . \] (38)

Substituting it into the original Hamiltonian (34), we see that this change of coordinates concerns only the first and second terms,
\[ -\frac{\hbar^2}{2m_-} \frac{\partial^2}{\partial z_-^2} - \frac{\hbar^2}{2m_+} \frac{\partial^2}{\partial z_+^2} = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial z_{cm}^2} - \frac{\hbar^2}{2m_\pm} \frac{\partial^2}{\partial z^2} = \frac{P_{\perp}^2}{2M} + \frac{p_{\perp}^2}{2m_\pm} , \] (39)
where \( p_z = -i\hbar \partial/\partial z \) and \( P_z = -i\hbar \partial/\partial z_{cm} \) are the relative and total longitudinal momenta, respectively, and
\[ m_\pm = m_\pm M/M \] (39)
is the reduced mass. Therefore we can fix the eigenvalue of the total longitudinal momentum \( P_z \) and write the total wave function and energy as
\[ \Psi_\pm(r_\perp, r_-, z, z_{cm}) = e^{iP_z z_{cm}/\hbar} \psi_\pm(r_\perp, r_-, z, z_{cm}) , \]
\[ E_{tot} = E + \frac{\hbar^2 P_{\perp}^2}{2M} . \] (40)
To find \( \psi(r_{+,-}, r_{-,-}, z) \), it is sufficient to consider the system that does not move along \( B \). Thus we will assume \( \hat{z} = 0 \) hereafter.

The wave function \( \psi \) and energy \( E \) satisfies the Schrödinger equation with the Hamiltonian

\[
H = \frac{p_r^2}{2m_s} + H_{\perp} + V_C. \tag{41}
\]

As follows from Sect. 11A the Landau functions

\[
\Phi_{n_{-} s_{-}}^{-1}(r_{-,-}) = (-1)^{s_{-}} \Phi_{n_{-} s_{-} r_{-,-}}^{(1)}(r_{-,-}) \quad \text{and} \quad \Phi_{n_{+} s_{+}}^{-1}(r_{+,-}) \quad \text{are eigenfunctions of the operators} \quad \pi_{-,-}^2 \quad \text{and} \quad \pi_{+,+}^2,
\]

so that

\[
\pi_{-,-}^2 \Phi_{n_{-} s_{-}}^{-1}(r_{-,-}) = \frac{\hbar^2}{a_m^2} (2n_{-} - 1) \Phi_{n_{-} s_{-}}^{-1}(r_{-,-}), \tag{42}
\]

\[
\pi_{+,+}^2 \Phi_{n_{+} s_{+}}^{-1}(r_{+,-}) = \frac{\hbar^2}{a_m^2} (2n_{+} + 1) \Phi_{n_{+} s_{+}}^{-1}(r_{+,-}), \tag{43}
\]

where \( n_{\pm} \geq 0 \) and \( s_{\pm} \geq -n_{\pm} \) are integer quantum numbers. Therefore, the transverse energy of two non-interacting particles, corresponding to the Hamiltonian \( H_{\perp} \), Eq. (45), is

\[
E_{n_{-} s_{-} n_{+} s_{+}}^{+} = \hbar \omega_{\perp} \left( n_{+} + \frac{1}{2} \right) + \hbar \omega_{\perp} \left( n_{-} + \frac{1}{2} \right), \tag{44}
\]

where

\[
\omega_{\perp} = \frac{eB}{m_c}, \quad \omega_{\perp} = \frac{ZeB}{m_c}. \tag{45}
\]

Since the eigenenergy (44) is degenerate with respect to quantum numbers \( s_{+} \) and \( s_{-} \), there is a manifold of eigenfunctions of representations of eigenfunctions, one of the simplest being

\[
\psi_{n_{+} s_{+} n_{-} s_{-} r_{+,-} (r_{+,-})} = \Phi_{n_{+} s_{+}}^{(2)}(r_{+,-}) \Phi_{n_{-} s_{-}}^{(-1)}(r_{-,-}). \tag{46}
\]

In addition, the wave function (16) is an eigenfunction of operators \( k_{-,-}^2 \) and \( k_{+,+}^2 \),

\[
k_{-} = p_{-} - \frac{e}{2c} B \times r_{-}, \quad k_{+} = p_{+} + \frac{ZeB}{2c} \times r_{+}, \tag{47}
\]

are pseudomomentum operators, and an eigenfunction of the operators of the \( z \)-projections of the angular momenta \( l_{-,-} \) and \( l_{+,+} \). Therefore, any set of commuting operators \( \pi_{-,-}^2, \pi_{+,+}^2 \), \( k_{-,-}^2, k_{+,+}^2 \), \( \pi_{-,-}^2, \pi_{+,+}^2, \pi_{-,-}^2, k_{+,+}^2, l_{-,-}, l_{+,+} \), \( \pi_{-,-}^2, \pi_{+,+}^2, l_{-,-}, l_{+,+} \) can be used for determination of the quantum numbers \( n_{+}, s_{+}, n_{-}, s_{-} \).

However, the basis (16) is not optimal, because the above sets of operators do not commute with our Hamiltonian (11), which means that the four quantum numbers \( n_{+}, s_{+}, n_{-}, s_{-} \) are not “good” in the presence of the Coulomb potential \( V_C \).

On the other hand, there are operators, which commute with each other and with the Hamiltonian \( H \): the total pseudomomentum

\[
k_{\text{tot}} = k_{-} + k_{+}, \tag{48}
\]

which is conserved due to translational invariance of \( H \) accompanied by the translational gauge transformations of \( A \) and the longitudinal component of the total angular momentum \( L_{z} = l_{-,-} + l_{+,+} \) (which is conserved because the potential \( V_C \) is rotationally invariant). For a charged system, the transverse Cartesian components of \( k_{\text{tot}} \) ( \( k_{\text{tot},x} \) and \( k_{\text{tot},y} \)) do not commute with each other and cannot be fixed simultaneously. Instead of selecting one of them, we may consider the square of pseudomomentum \( k_{z}^2 \). Thus we look for common eigenfunctions of commuting operators \( \pi_{-,-}^2, \pi_{+,+}^2, k_{\text{tot},z}^2 \), and \( L_z \), which will serve as a basis, corresponding to two integrals of motion of our system, because two operators of this set commute with the Hamiltonian.

Unlike the system of particles without external fields, the center-of-mass coordinates of the system of charged particles in a magnetic field cannot be completely eliminated from the Hamiltonian. When an external magnetic field is present, the collective behaviors of a neutral system of charged particles, such as an atom, and of a charged system, such as an atomic ion, are very different. In the former case, the collective motion is free whereas in the latter case, a cyclotron motion arises. This difference appears clearly in the detailed mathematical study of Avron et al. [23]. 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. Thus the set of operators \( (k_{z}^2, L_z) \) is not exclusively associated with the collective motion but involves both the collective and internal degrees of freedom.

One can, however, perform an approximate separation in the form \( H = H_1 + H_2 + H_3 \), where Hamiltonians \( H_1 \) and \( H_2 \) describe the motion of quasiparticles corresponding to the collective and internal degrees of freedom, respectively, and operator \( H_3 \) couples the internal and collective phase coordinates. An example of such approximate separation was presented by Schmelcher & Cederbaum [24, 27], who applied a canonical transformation of variables to the Hamiltonian written in terms of the center-of-mass and relative coordinates of the particles. Baye and Vincke [3] developed a general framework for approximate separations. They introduced a parametrized approximate collective integral of motion, which in the two-particle case has the form

\[
C(\alpha_1) = k_{\text{tot},z} - (Z - 1) (e/c) B \times (a_0 r_{-,-} + a_1 r_{-,-}), \tag{49}
\]

where \( a_0 = 1 - \alpha_1 \) and \( \alpha_1 \) is a free parameter.

In the following we will assume that \( m_{+} \gg m_{-} \). Baye and Vincke [3] have shown that in this case any choice of \( \alpha_1 \) will provide the approximate separation as long as \( \alpha_1 = O(m_{-}/m_{+}) \). The simplest choice \( \alpha_1 = 0 \) has been introduced by Baye [28] and successfully used by Baye and Vincke [29] in the calculations of the collective motion corrections for atomic ions.
However, since the separation of the collective motion is only approximate, there is no particular advantage in selecting the center of mass for describing the coordinate of the quasiparticle corresponding to the collective motion. An equally reasonable choice can be just the coordinate of the heavy particle (the nucleus). Using the latter choice, Bezchastnov [18] derived a basis of eigenstates of the transverse Hamiltonian \( H_\perp \), whose elements are also eigenstates of squared total pseudomomentum \( K^2 \), total \( z \)-projection of the angular momentum \( L_z \), and squared kinetic momenta of each particle, \( \pi^2_\perp \) and \( \pi^2_\perp \). In Sect. III we present a more detailed and physically transparent derivation of the same basis with some corrections.

III. TRANSVERSE BASIS

A. Canonical transformations

Let us pass from variables \((r_{+\perp}, r_{-\perp})\) to variables \((R_\perp, r_\perp)\), where

\[
R_\perp = r_{+\perp}, \quad r_\perp = r_{-\perp} - r_{+\perp}.
\]

Hereafter we will also use the three-dimensional vectors \( R \) and \( r \), assuming the \( z \)-components \( R_z = 0 \) and \( r_z = z \), so that \( r = r_\perp - r_{+\perp} \). The canonical momenta transform as

\[
p_+ = P - p, \quad p_- = p.
\]

In the new variables, the transverse Hamiltonian becomes

\[
H_\perp = \frac{1}{2m_+} \left( P_\perp - p_\perp - \frac{Ze}{2c} B \times R \right)^2 + \frac{1}{2m_-} \left( p_\perp + \frac{e}{2c} B \times r + \frac{e}{2c} B \times R \right)^2.
\]

The total pseudomomentum \[\text{Eq. (52)}\] becomes

\[
k_{\text{tot}} = P + \frac{(Z-1)e}{2c} B \times R - \frac{e}{2c} B \times r.
\]

We look for a unitary transformation, which will allow us to separate motion of quasiparticles with the total charge of the system, \((Z-1)e\), and with the electron charge, \(-e\). For this aim, we should transform the first bracket so as to add \((e/2c) B \times R\) in it, and the second bracket so as to subtract \((e/2c) B \times R\). The unitary transformation operator can be written in the form \( U = \exp(-i\phi) \), where \( \phi \) is a Hermittian operator to be determined. The wave function is transformed as \( \psi = U \psi' \), \( \psi' = U^\dagger \psi \), and the Hamiltonian as \( H = U H' U^\dagger \), \( H' = U^\dagger H U \) (symbol \( U^\dagger \) denotes the Hermittian adjoint to \( U \)). It is easy to check that for our purpose we can take

\[
U = \exp \left( -\frac{ie}{2\hbar c} (B \times r) \cdot R \right)
\]

\[
= \exp \left( -\frac{ie}{2\hbar c} (B \times r_-) \cdot r_+ \right)
\]

\[
= \exp \left( \frac{ie}{2\hbar c} (B \times r_+) \cdot r_- \right).
\]

This operator performs a gauge transformation and shifts the momenta:

\[
U^\dagger P U = P + \frac{e}{2c} B \times r, \quad U^\dagger p U = p - \frac{e}{2c} B \times R.
\]

This shift cancels the third term in Eq. \[\text{52}\], and the total pseudomomentum becomes

\[
K = U^\dagger k_{\text{tot}} U = P + \frac{(Z-1)e}{2c} B \times R.
\]

The total angular momentum \( L = l_- + l_+ = r_+ \times p_+ + r_- \times p_- = R \times P + r \times p \) retains its form after the transformation: \( U^\dagger L U = L \). The operators of kinetic momenta of the nucleus and the electron become respectively

\[
U^\dagger \pi_k U = \Pi - k, \quad U^\dagger \pi_- U = \pi.
\]

where

\[
\Pi = P - \frac{(Z-1)e}{2c} B \times R, \quad \pi = p + \frac{e}{2c} B \times r,
\]

\[
k = p - \frac{e}{2c} B \times r.
\]

Therefore the transformed transverse Hamiltonian equals

\[
H'_\perp = U^\dagger H_\perp U = \frac{1}{2m_+} (\Pi_\perp - k_\perp)^2 + \frac{\pi^2_\perp}{2m_-}.
\]

We will consider \( \Pi \) and \( \pi \) as kinetic momenta of quasiparticles with charges \((Z-1)e\) and \((-e)\), and \( k \) as a pseudomomentum of the latter quasiparticle. By analogy with Eq. \[\text{5}\], the \( z \)-projection of the total angular momentum \[\text{Eq. (59)}\] equals

\[
L_z = \frac{c}{2(Z-1)eB} (K^2_\perp - \Pi^2_\perp) + \frac{c}{2eB} (\pi^2_\perp - k^2_\perp).
\]

Expanding the brackets in Eq. \[\text{59}\] and substituting \( k^2_\perp = \pi^2_\perp - (2eB/c) l_z \), we obtain

\[
H'_\perp = H'_1 + H'_2 + H'_3,
\]

where

\[
H'_1 = \frac{\Pi^2_\perp}{2m_+}, \quad H'_2 = \frac{\pi^2_\perp}{2m_-},
\]

\[
H'_3 = -\frac{1}{m_+} \Pi_\perp \cdot k - \frac{eB}{m_+c} l_z.
\]
Here, we have introduced the $z$-projection $l_z$ of the angular momentum of the second (negative) quasiparticle by analogy with Eq. (53). The term $m_{-1}^2 \Pi_\perp \cdot k_\perp$ in $H'_3$ couples together the motion of the two quasi-particles.

Equivalently, $k$ and $\pi$ might be considered as the kinetic momentum and pseudomomentum of a quasiparticle with charge $+e$. Accordingly, the transverse Hamiltonian can be rewritten as

$$H'_\perp = H'_1 + H'_2 + H''_2,$$  \hspace{1cm} (64)

where $H'_1$ is the same as in Eq. (62) and

$$H''_2 = \frac{k^2}{2m_*}, \quad H''_3 = -\frac{1}{m^*} \Pi_\perp \cdot k_\perp + \frac{eB}{m_c} l_z.$$  \hspace{1cm} (65)

Comparing the last formula with Eq. (63), we see that $H''_2 = H'_3 + (eB/m_{\text{ext}}) l_z$. The latter decomposition (64) was used in Ref. [18]. We prefer to use the former decomposition, Eq. (64), because $H'_1 \to 0$ at $m^* \to \infty$, ensuring asymptotic decoupling for massive ions.

Operators $H'_1$ and $H'_2$ ($H''_2$) have the form of the Hamiltonian of free quasiparticles with charges $(Z - 1)e$ and $e$ ($-e$) and masses $m_+$ and $m_*$, respectively. And $H'_3$ ($H''_3$) couples them together. According to Sect. II A, the eigenfunctions of $H'_1$ are $\Phi_{\pi_1}(r_\perp)$, $N \geq 0$, $S \geq -N$, and the eigenenergies are independent of $S$,

$$E_{1,N} = \hbar \omega_{c_1} \left( N + \frac{1}{2} \right),$$  \hspace{1cm} (66)

where

$$\omega_{c_1} = \frac{(Z - 1)eB}{m_+ c} = \frac{Z - 1}{Z} \omega_{c_+}.$$  \hspace{1cm} (67)

Analogously, the eigenfunctions of $H'_2$ are $\Phi_{\pi_1}(r_\perp)$, $n \geq 0$, $s \geq -n$, and the eigenenergies are independent of $s$,

$$E_{2,n} = \hbar \omega_{c_2} \left( n + \frac{1}{2} \right),$$  \hspace{1cm} (68)

where

$$\omega_{c_2} = \frac{eB}{m_* c} = \left( 1 + \frac{m_-}{m_+} \right) \omega_{c_-}.$$  \hspace{1cm} (69)

**B. Creation and annihilation operators**

Instead of $S$ and $s$, it is sometimes convenient to use quantum numbers $\tilde{N} = N + S$ and $\tilde{n} = n + s$. As follows from Eq. (21), an interchange of $n$ with $\tilde{n}$ or $N$ with $\tilde{N}$ does not affect the modulus of a single-particle eigenfunction. We will use these quantum numbers to specify quantum states $|N, \tilde{N}\rangle$ and $|n, \tilde{n}\rangle$ of the two quasiparticles, described by Hamiltonians $H'_1$ and $H'_2$, respectively, in the $(xy)$-plane.

Let us consider the cyclic components (61) of the operators of the kinetic momenta and pseudomomenta of the quasiparticles. According to Eqs. (32) and (33), the operators

$$\hat{a} = i \frac{a_m}{\hbar} \pi_{-1}, \quad \hat{\pi} = -i \frac{a_m}{\hbar} \pi_{+1},$$  \hspace{1cm} (70a)

$$\hat{b} = i \frac{a_m}{\hbar} \Pi_{-1}, \quad \hat{\pi} = -i \frac{a_m}{\hbar} \Pi_{+1},$$  \hspace{1cm} (70b)

lower the quantum numbers $n, \tilde{n}, N, \tilde{N}$ by one, as follows:

$$\hat{a} |n, \tilde{n}\rangle = \sqrt{n} |n - 1, \tilde{n}\rangle,$$  \hspace{1cm} (71a)

$$\hat{b} |N, \tilde{N}\rangle = \sqrt{N} |N - 1, \tilde{N}\rangle.$$  \hspace{1cm} (71c)

Their Hermitian adjoint operators

$$\hat{a}^\dagger = -i \frac{a_m}{\hbar} \pi_{+1}, \quad \hat{\pi}^\dagger = \frac{a_m}{\hbar} \pi_{-1},$$  \hspace{1cm} (72a)

$$\hat{b}^\dagger = -i \frac{a_m}{\hbar} \Pi_{+1}, \quad \hat{\pi}^\dagger = -i \frac{a_m}{\hbar} \Pi_{-1},$$  \hspace{1cm} (72b)

raise the quantum numbers $n, \tilde{n}, N, \tilde{N}$ by one:

$$\hat{a}^\dagger |n, \tilde{n}\rangle = \sqrt{n + 1} |n + 1, \tilde{n}\rangle,$$  \hspace{1cm} (73a)

$$\hat{b}^\dagger |N, \tilde{N}\rangle = \sqrt{N + 1} |N + 1, \tilde{N}\rangle.$$  \hspace{1cm} (73c)

As far as $\hat{a}, \hat{a}^\dagger, \hat{b}, \hat{b}^\dagger$ can be considered as annihilation operators for excitations in $n, \tilde{n}, N, \tilde{N}$, their Hermitian adjoint operators can be considered as the creation operators.

It is noteworthy that

$$\pi_{\pm 1} = \pm \frac{ieB}{2c} r_{\pm 1},$$  \hspace{1cm} (74)

$$K_{\pm 1} = \pm \frac{ieB}{2c} r_{\pm 1},$$  \hspace{1cm} (75)

$$\Pi_{\pm 1} = \pm \frac{i(Z - 1)eB}{2c} R_{\pm 1},$$  \hspace{1cm} (76)

$$K_{\pm 1} = \pm \frac{i(Z - 1)eB}{2c} R_{\pm 1}.$$  \hspace{1cm} (77)

Therefore,

$$r_{\pm 1} = \pm \frac{ic}{eB} (k_{\pm 1} - \pi_{\pm 1}),$$  \hspace{1cm} (78)

$$R_{\pm 1} = \pm \frac{ic}{(Z - 1)eB} (K_{\pm 1} - \Pi_{\pm 1}),$$  \hspace{1cm} (79)

so that

$$r_{+1} = a_m (\hat{a}^\dagger - \hat{\pi}^\dagger), \quad r_{-1} = a_m (\hat{a} - \hat{\pi})$$  \hspace{1cm} (80a)

$$R_{+1} = a_m z_{-1} (\hat{b}^\dagger - \hat{\pi})^\dagger, \quad R_{-1} = a_m z_{-1} (\hat{b} - \hat{\pi})^\dagger.$$  \hspace{1cm} (80b)

It is also useful to consider the circular components of the kinetic momentum of the nucleus $\pi_+$. According
to Eq. (62), these operators change the nucleus Landau number \( n_+ \) by \( \pm 1 \):

\[
\pi_{+,+1} |n_+ \rangle = - \frac{i \hbar}{a_{m,z}} \sqrt{n_+} |n_+ - 1, \tilde{n}_+ \rangle,
\]

\[
\pi_{+,-1} |n_+ \rangle = \frac{i \hbar}{a_{m,z}} \sqrt{n_+ + 1} |n_+ + 1, \tilde{n}_+ \rangle.
\]

(81a)  

(81b)

The canonical transformation of these operators with account of Eq. (57) and Eqs. (70), (72) gives

\[
U^\dagger \pi_{+,+1} U = \Pi_{+,+1} - k_{+,+1} = - \frac{i \hbar}{a_m} (\sqrt{Z - 1} \hat{b} + \hat{a}),
\]

\[
U^\dagger \pi_{+,-1} U = \Pi_{-,+1} - k_{-,+1} = \frac{i \hbar}{a_m} (\sqrt{Z - 1} \hat{b} + \hat{a}^\dagger).
\]

(82a)  

(82b)

C. Good quantum numbers

The effective quasiparticle Hamiltonians can be written in terms of the creation and annihilation operators (Sect. III B) as

\[
H'_1 = \hbar \omega_{c_1} \left( \hat{b}^\dagger \hat{b} + \frac{1}{2} \right), \quad H'_2 = \hbar \omega_{c_2} \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right).
\]

(83)

Using the expressions \( l_z = \hbar (\hat{a}^\dagger \hat{a} - \hat{\bar{a}} \hat{\bar{a}}) \) and

\[
\Pi_{\perp} \cdot k_{\perp} = \frac{-\hbar^2}{a_m^2} \sqrt{Z - 1} (\hat{\bar{a}} \hat{\bar{a}} - \hat{\bar{a}}^\dagger \hat{\bar{a}}),
\]

we can write the coupling operator \( H'_3 \) in Eq. (63) as

\[
H'_3 = \frac{\hbar \omega_{c_1}}{\sqrt{Z - 1}} (\hat{\bar{a}} \hat{\bar{a}} - \hat{a}^\dagger \hat{a}) + \frac{\hbar \omega_{c_2}}{\sqrt{Z - 1}} (\hat{a}^\dagger \hat{a} - \hat{\bar{a}} \hat{\bar{a}}).
\]

(85)

Equations (83) and (85) do not contain operators \( \hat{b}' \) and \( \hat{b}'^\dagger \), which determine the square of total transverse pseudomomentum

\[
K^2_{\perp} = \frac{2 \hbar^2}{a_m^2} (Z - 1) (\hat{b}^\dagger \hat{b} + \frac{1}{2}),
\]

(86)

which confirms that \( K^2_{\perp} \) is an integral of motion ([\( H'_1, K^2_{\perp} \) = 0] and the related quantum number \( \tilde{N} = \langle \hat{b}^\dagger \hat{b} \rangle \) is conserved. In other words, \( \tilde{N} \) is a good quantum number.

For the \( z \)-projection of the total angular momentum, Eq. (60) gives

\[
L_z = \hbar (\hat{b}^\dagger \hat{b} - \hat{b} \hat{b}^\dagger + \hat{a}^\dagger \hat{a} - \hat{\bar{a}} \hat{\bar{a}}).
\]

(87)

The eigenvalues of \( L_z \) equal \( \hbar L = \hbar (S - \bar{s}) \). It is easy to check that \( [H'_1, L_z] = 0 \). Therefore, \( L \) is a good quantum number. From Eq. (87) we see that

\[
L = \tilde{N} - \tilde{N} - \tilde{n} + n.
\]

(88)

Finally, using Eqs. (83), (85), and the expression

\[
\pi_{\perp}^2 = \frac{\hbar^2}{a_m^2} (2 \hat{\bar{a}} \hat{\bar{a}} + 1),
\]

(89)

we can check that \( [\pi_{\perp}^2, H'_1] = 0 \). It means that \( n = \langle \hat{a}^\dagger \hat{a} \rangle \) is a good quantum number (as long as we disregard \( V_C \)).

D. Transverse basis states

The results of Sect. III C allow us to consider eigenstates of the transverse Hamiltonian \( H'_{\perp} \) with fixed numbers \( N, n, L \). On the other hand, the quantum numbers \( S \) and \( s = S - L \), or equivalently \( N = \tilde{N} - S \) and \( n = n + s \) are not well defined, because \( l_z \) does not commute with \( H'_3 \). Since the eigenfunctions \( \mathcal{F}^{(2-1)}_{N, \tilde{N}, n, \tilde{n}}(R_{\perp}) \mathcal{F}^{(-1)}_{n, \tilde{n}}(r_{\perp}) \) of the states \( |N, \tilde{N}, n, \tilde{n} \rangle = |N, \tilde{N}, \rangle \otimes |n, \tilde{n} \rangle \) with fixed \( N \) and \( n \) (recall that \( |N, \tilde{N} \rangle \) and \( |n, \tilde{n} \rangle \) are the eigenstates of \( H'_1 \) and \( H'_2 \), respectively) form a complete basis in the Hilbert space of functions of \( (R_{\perp}, r_{\perp}) \), the eigenstates of \( H'_{\perp} \) can be looked as superpositions of states \( |N, \tilde{N}, n, \tilde{n} \rangle \) with different \( N \) and \( \tilde{N} \). Taking into account the constraint \( N + \tilde{n} = \tilde{N}, \) where \( N \equiv \tilde{N} - L + n \), we can write the eigenfunction \( \Psi' = U \Psi \) of \( H'_{\perp} \) as

\[
\Psi'_{N, n, L}(R_{\perp}, r_{\perp}) = \sum_{\tilde{n}=0}^{N} C_{\tilde{n}} \mathcal{F}^{(2-1)}_{N - \tilde{n}, \tilde{N}}(R_{\perp}) \mathcal{F}^{(-1)}_{n, \tilde{n}}(r_{\perp}),
\]

(90)

where \( C_{\tilde{n}} \) are some constants, which may depend on \( \tilde{N}, n, L \). The eigenfunctions of the initial Hamiltonian \( H_{\perp} \) are

\[
\Psi_{\tilde{N}, n, L}(r_{\perp}, r_{-\perp}) = U \sum_{\tilde{n}=0}^{N} C_{\tilde{n}} \mathcal{F}^{(2-1)}_{N - \tilde{n}, \tilde{N}}(r_{\perp, + \perp}) \mathcal{F}^{(-1)}_{n, \tilde{n}}(r_{- \perp, + \perp}),
\]

(91)

where \( U \) is given by Eq. (63).

By construction, \( \Psi_{\tilde{N}, n, L}(r_{\perp, + \perp}, r_{- \perp, + \perp}) \) is an eigenfunc-

tion of \( L_z \) and \( K^2 \) for any coefficients \( C_{\tilde{n}} \). Let us consider its transformation under the action of operators \( \pi_{\perp}^2 \).
Equation (59) gives
\[ \pi_\perp^2 \ket{N, \tilde{N}, n, \tilde{n}} = \frac{\hbar^2}{a_m^2} (2n + 1) \ket{N, \tilde{N}, n, \tilde{n}}. \] (92)

On the other hand, according to Eq. (57), \( \pi_\perp^2 = U^\dagger \pi_\perp^2 U \). Therefore, \( \Psi_{\tilde{N}, n, L}(r_{+\perp}, r_{-\perp}) \) is an eigenfunction of \( \pi_{\perp}^2 \) with the appropriate eigenvalue \( (\hbar/a_m)^2 (2n + 1) \) for any set of \( C_R \), which means that \( n_- = n \). Therefore, we can write
\[ \mathcal{N} = \tilde{N} - L + n_- \] (93)

The operator \( \pi_{+\perp}^2 \), being transformed according to Eq. (57), can be expressed using Eq. (54) as
\[ (\Pi_\perp - k_\perp)^2 = \frac{\hbar^2}{a_m^2} \left[ 2(Z - 1)(\hat{b}^\dagger \hat{b} + 1) + 2\hat{a}^\dagger \hat{a} + 1 \right]. \] (94)

From this equation, taking into account that \( N = \mathcal{N} - \tilde{n} \), we obtain
\[ (\Pi_\perp - k_\perp)^2 \ket{N, \tilde{N}, n, \tilde{n}}_\perp = \frac{2\hbar^2}{a_m^2} \left[ (Z - 1)(\mathcal{N} - (Z - 2)\tilde{n} + \frac{Z}{2}) \ket{N - \tilde{n}, \tilde{N}, n, \tilde{n}}_\perp + \sqrt{Z - 1} \sqrt{(\mathcal{N} - \tilde{n})(\tilde{n} + 1)} \ket{N - \tilde{n} - 1, \tilde{N}, n, \tilde{n} + 1}_\perp + \sqrt{Z - 1} \sqrt{(\mathcal{N} - \tilde{n} + 1)\tilde{n} \mathcal{N} - n + 1, \tilde{N}, n, \tilde{n} - 1}_\perp \right]. \] (95)

Using this relation with Eq. (90) and changing the summation index \( \tilde{n} \) so as to collect together the homogeneous terms with \( f_{\mathcal{N} - \tilde{n}, \tilde{N}}(R_\perp)f_{n, \tilde{n}}^{(-1)}(r_\perp) \), we obtain
\[ (\Pi_\perp - k_\perp)^2 \Psi_{\tilde{N}, n, L}(R_\perp, r_\perp) = \frac{2\hbar^2}{a_m^2} \sum_{\tilde{n} = 0}^{N} \left[ (Z - 1)(\mathcal{N} - (Z - 2)\tilde{n} + \frac{Z}{2}) C_{\tilde{n}} + \sqrt{Z - 1} \sqrt{(\mathcal{N} - \tilde{n} + 1)\tilde{n} \mathcal{N} - n + 1, \tilde{N}, n, \tilde{n} + 1}_\perp \right] f_{\mathcal{N} - \tilde{n}, \tilde{N}}(R_\perp)f_{n, \tilde{n}}^{(-1)}(r_\perp). \] (96)

Comparing Eq. (96) with Eq. (90), we see that \( \Psi_{\tilde{N}, n, L}(R_\perp, r_\perp) \) will be an eigenfunction of \( (\Pi_\perp - k_\perp)^2 = U^\dagger \pi_{+\perp}^2 U \) under the condition that the coefficients \( C_{\tilde{n}} \) satisfy the relation (41)
\[ \sqrt{Z - 1} \left[ \sqrt{(\mathcal{N} - \tilde{n} + 1)\tilde{n} C_{\tilde{n}} - 1} + \sqrt{(\mathcal{N} - \tilde{n})(\tilde{n} + 1)} C_{\tilde{n} + 1} \right] = [(Z - 2) \tilde{n} - (Z - 1)\mathcal{N} + Zn_+] C_{\tilde{n}}, \] (97)

where \( n_+ = 0, 1, 2, \ldots, \mathcal{N} \). Imposing this relation, we see from Eq. (96) that
\[ \pi_{+\perp}^2 \Psi_{\tilde{N}, n, L}(r_{+\perp}, r_{-\perp}) = \frac{2\hbar^2}{a_m^2} \left( n_+ + \frac{1}{2} \right) \Psi_{\tilde{N}, n, L}(r_{+\perp}, r_{-\perp}), \] (98)

Each value of \( n_+ \) corresponds to an eigenvector \( \{ C_{\tilde{n}} \} (\tilde{n} = 0, 1, \ldots, \mathcal{N}) \). We see that the numbers \( \tilde{N}, n = n_- \), and \( L \) affect the eigenvalue problem only in combination \( \mathcal{N} = \tilde{N} + n_- - L \). Therefore each eigenvector may be marked by only two numbers \( \mathcal{N} \) and \( n_+ \). These eigenvectors are orthonormal,
\[ \sum_{k=0}^{\mathcal{N}} C_k^{(\mathcal{N}, n_+)} C_k^{(\mathcal{N}, n_+)} = \delta_{n_+'n_+}, \] (99)

therefore they form an orthonormal basis in a \((\mathcal{N} + 1)\)-dimensional vector space.

Thus we have built a basis of eigenstates of four oper-
The states \(|\tilde{N}, L, n_-, n_+\rangle\) are characterized by 4 discrete quantum numbers, related to the four degrees of freedom for motion of the 2 charged particles perpendicular to the magnetic field:

\[
K_z^2 |\tilde{N}, L, n_-, n_+\rangle \perp, 0 = \frac{\hbar^2}{a_{m, Z-1}^2} (2\tilde{N} + 1) |\tilde{N}, L, n_-, n_+\rangle \perp, 0,
\]

\[
L_z |\tilde{N}, L, n_-, n_+\rangle \perp, 0 = \hbar L |\tilde{N}, L, n_-, n_+\rangle \perp, 0,
\]

\[
\pi_\perp^2 |\tilde{N}, L, n_-, n_+\rangle \perp, 0 = \frac{\hbar^2}{a_{m}^2} (2n_- + 1) |\tilde{N}, L, n_-, n_+\rangle \perp, 0,
\]

\[
\pi_\perp^2 |\tilde{N}, L, n_-, n_+\rangle \perp, 0 = \frac{\hbar^2}{a_{m}^2} (2n_+ + 1) |\tilde{N}, L, n_-, n_+\rangle \perp, 0,
\]

\[
\tilde{N} \geq 0, \quad n_- \geq 0, \quad L \leq \tilde{N} + n_-, \quad 0 \leq n_+ \leq \tilde{N} = \tilde{N} + n_- - L.
\]

According to Eqs. (35), (103), and (106),

\[
H \perp |\tilde{N}, L, n_-, n_+\rangle \perp, 0 = E_{n_-, n_+}^{\perp} |\tilde{N}, L, n_-, n_+\rangle \perp, 0,
\]

where \(E_{n_-, n_+}^{\perp}\) is defined by Eq. (44). This basis is orthonormal,

\[
\langle \tilde{N}', L', n'_-, n'_+ |\tilde{N}, L, n_-, n_+\rangle \perp, 0 = \delta_{\tilde{N}' \tilde{N}} \delta_{L' L} \delta_{n'_- n_-} \delta_{n'_+ n_+}
\]

and complete,

\[
\sum_{\tilde{N}, L, n_-, n_+} \Psi_{\tilde{N}, L, n_-, n_+} (r_+, \perp, r_-, \perp) \Psi_{\tilde{N}, L, n_-, n_+} (r_-, \perp, r_+, \perp) = \delta (r_+ \perp - r_+ \perp) \delta (r_- \perp - r_- \perp).
\]

Using Eq. (39), one can rewrite Eq. (102) in the form

\[
\Psi_{\tilde{N}, L, n_-, n_+} (r_+, \perp, r_-, \perp) = U^\dagger \sum_{\tilde{n} = 0}^{\tilde{N}} \left(-1\right)^{n_- - \tilde{n}} C_{\tilde{n}}^{(N, n_+)} F_{\tilde{n}, \tilde{N}}^{(Z-1)} (r_+, \perp) F_{\tilde{n}, n_-}^{(1)} (r_- \perp),
\]

which is equivalent to the representation used in Ref. [18].

### E. Recurrence relations for the basis coefficients

Equation (107) can be rewritten in the form

\[
\sqrt{(\tilde{N} - \tilde{n} + 1)} \tilde{n} C_{\tilde{n}}^{(N, n_+)} + \sqrt{(\tilde{N} - \tilde{n})(\tilde{n} + 1)} C_{\tilde{n} + 1}^{(N, n_+)} = \frac{Z (\tilde{n} + n_+ - \tilde{N}) - 2\tilde{n} + \tilde{N}}{\sqrt{Z - 1}} C_{\tilde{n}}^{(N, n_+)}
\]

and used as a recurrence relation to calculate the coefficients \(C_{\tilde{n}}^{(N, n_+)}\) for given values of \(\tilde{N}\) and \(n_+\). One can start the recurrent procedure from an arbitrary value of the initial coefficient to (for instance \(C_{0}^{(N, n_+)} = 1\) for the upward...
recurrence of $C^{(N, n_+)} = 1$ for the downward recurrence), and then scale them by a single number factor to satisfy the normalization relation
\begin{equation}
\sum_{\hat{n}=0}^{N} \left| C^{(N, n_+)}_{\hat{n}} \right|^2 = 1,
\end{equation}
(113)
The upward recurrence (that is, starting from $\hat{n} = 0$ to higher $\hat{n}$) is stable under the condition that it is performed for $n_+ \geq N - Z$, whereas the downward recurrence (starting from $\hat{n} = N$ to lower $\hat{n}$) is stable for $n_+ < N - Z$.

Supplementary recurrence relations for coefficients $C^{(N, n_+)}_{\hat{n}}$ are derived in Appendix A.

### IV. SOLUTION OF THE SCHRODINGER EQUATION

#### A. Expansion on the transverse basis

We are looking for eigenfunctions of Hamiltonian $H$ in Eq. (31). The potential $V_C$ commutes with the transformed total pseudomomentum $K$ [Eq. (55)] and the total angular momentum $L$ [Eq. (56)]. Therefore, we may consider states with definite $K^2$ and $L_\perp$, that is to fix $\tilde{N}$ and $L$. However, $V_C$ does not commute with squared kinetic momenta $p^2$. Let us expand the states with fixed $\tilde{N}$ and $L$ over the complete basis of states constructed in Sect. III D:

\begin{equation}
\psi_\kappa (r_{+, \perp}, r_{-, \perp}, z) = \sum_{n_-, n_+} \Psi_{\tilde{N}, L, n_-, n_+} (r_{+, \perp}, r_{-, \perp}) g_{n_- n_+; \kappa} (z).
\end{equation}
(114)

Here $\kappa$ is a compound quantum number, which is assigned to the considered quantum state and includes $\tilde{N}$ and $L$. Let us substitute Eq. (114) into the Schrödinger equation
\begin{equation}
H \psi_\kappa = E_\kappa \psi_\kappa,
\end{equation}
(115)
multiply both sides by $\Psi^*_{\tilde{N}, L, n_-, n_+} (r_{+, \perp}, r_{-, \perp})$, and integrate over $r_{+, \perp}, r_{-, \perp}$. Using Eqs. (34), (108), and (109), we obtain
\begin{equation}
\left( \frac{\hbar^2}{2m_\perp} - E^\perp_{\kappa} \right) g_{n_- n_+; \kappa} (z) = - \sum_{n'_-, n'_+} \sum_{n_-, n_+} V^{(\tilde{N} - L)}_{n'_-, n'_+; n_- n_+} (z) g_{n'_- n'_+; \kappa} (z),
\end{equation}
(116)
where
\begin{equation}
E^\perp_{\kappa} = E_\kappa - E^\perp_{n_-, n_+}
\end{equation}
(117)
is the energy corresponding to the relative motions along $z$ and
\begin{equation}
V^{(\tilde{N} - L)}_{n'_-, n'_+; n_- n_+} (z) = \sum_{k'=0}^{N'} \sum_{k=0}^{N} C^{(N', n'_+)}_{k'} C^{(N, n_+)}_k \int_{\mathbb{R}^2} \mathcal{F}^{(Z-1)*}_{N'-k', \tilde{N}} (R_{\perp}) \mathcal{F}^{(Z-1)}_{N-k, \tilde{N}} (R_{\perp}) dR_{\perp}
\times \int_{\mathbb{R}^2} \mathcal{F}^{(-1)*}_{n'_-, k'} (r_{\perp}) \frac{-Ze^2}{\sqrt{r^2 + z^2}} \mathcal{F}^{(-1)}_{n_- k} (r_{\perp}) dr_{\perp}
\end{equation}
(118)
is an effective one-dimensional potential, $\tilde{N}' = \tilde{N} - L + n'_-$, $\tilde{N} = \tilde{N} - L + n_-$. Since the Coulomb potential does not contain $R_{\perp}$, the first integral in Eq. (118) equals $\delta_{N'-k', \tilde{N}' - k'} = \delta_{k', n'_- - n_- + k}$. Thus, using Eq. (29), we obtain
\begin{equation}
V^{(\tilde{N} - L)}_{n'_-, n'_+; n_- n_+} (z) = \sum_{k=k_{\text{min}}}^{N} C^{(N', n'_+)}_{n'_-, n_- + k} C^{(N, n_+)}_k \int_{\mathbb{R}^2} \Phi^{(-1)*}_{n'_-, k'} (r_{\perp}) \frac{-Ze^2}{\sqrt{r^2 + z^2}} \Phi^{(-1)}_{n_- k} (r_{\perp}) dr_{\perp},
\end{equation}
(119)
$k_{\text{min}} = \max(0, n_- - n'_-)$. Since the transverse basis is complete, the infinite system (116) is equivalent to the Schrödinger equation (115). Truncating the sum (114), one obtains a finite system, which solves Eq. (115) approximately. The same finite system of equations can be obtained from the variational principle on the truncated basis.
B. Calculation of effective potentials

It is convenient to define reduced (dimensionless) potentials through the relations

\[
V^{(\mathcal{N} - L)}_{n',n'_+;n_-,n_+}(z) = \frac{-Ze^2}{a_m \sqrt{2}} v^{(\mathcal{N} - L)}_{n',n'_+;n_-,n_+}(\zeta), \quad \zeta = \frac{z}{a_m \sqrt{2}},
\]

where \(s_{\min} = -\min(n_-, n'_+),\)

\[
v_{n',n';s}(\zeta) = \sum_{s=s_{\min}}^{\infty} C^{(\mathcal{N}',n'_+)}_{n_+',s} C^{(\mathcal{N},n_+)}_{n_+,s} v_{n_+',n_+}(s)(\zeta),
\]

where \(s_{\min} = -\min(n_-, n'_+),\)

\[v_{n,k;s}(\zeta) = \frac{1}{n!(n+s)!l!(k+s)!} \sum_{l=0}^{n} \frac{1}{l!(n-l)!(l+s)!} \sum_{m=0}^{k} \frac{(-1)^m l s (s+l+m)!}{m l (k+m)! (s+m)!} v_{s+l+m}(\zeta),\]

and

\[v_s(\zeta) = \frac{1}{s!} \int_{0}^{\infty} x^s e^{-x} \frac{dx}{\sqrt{\zeta^2 + x}}.\]

A change of variable brings the latter integral to

\[v_s(\zeta) = \frac{1}{s!} \int_{\zeta^2}^{\infty} (x - \zeta^2)^s e^{\zeta^2 - x} \frac{dx}{\sqrt{x}} = \sum_{l=0}^{s} (-1)^l \frac{s! l!}{l!(s-l)!} \zeta^{2l} e^{\zeta^2} \Gamma(s - l + 1/2, \zeta^2),\]

where \(\Gamma(a,x)\) is the incomplete gamma function. At small or moderate \(\zeta, v_s(\zeta)\) can be calculated using the recurrence relation

\[v_{s+1}(\zeta) = (2s + 1) v_s(\zeta) + \frac{\zeta^2}{s + 1} \left[ v_{s-1}(\zeta) - v_s(\zeta) \right],\]

\[v_0(\zeta) = \sqrt{\pi} e^{\zeta^2} \text{erfc}(|\zeta|),\]

\[v_1(\zeta) = \frac{1 - 2\zeta^2}{2} v_0(\zeta) + |\zeta|.\]

Here, \(\text{erfc}(z)\) is the complementary error function, which can be calculated using, e.g., an expansion in power series at small \(|\zeta|\) and continued fractions at \(|\zeta| \geq 1\). At large \(|\zeta|\) or \(s\), however, the recurrence relation (128) fails because of round-off errors in positive and negative terms, which nearly annihilate. In this case, one can use the asymptotic formula

\[v_s(\zeta) \sim \frac{1}{\sqrt{\zeta^2 + 1} + s} \left( 1 + \frac{3}{8} \frac{1 + s}{\zeta^2 + 1 + s^2} \right).\]

C. Adiabatic approximation

In strong magnetic fields, such that \(\hbar \omega_{e-} \gg Z \omega\) (where \(\omega = m_e e^2/h^2\) is the atomic unit of energy), the system of equations (116) approximately splits into separate subsystems with fixed \(n_-\). Indeed, since the magnetic length \(a_m\) is small at large \(B\), the denominator \(C_{n,m}\) in Eq. (119) remains nearly constant over the range where the Landau functions \(\Phi\) in the integral are not too small. Since the Landau functions are orthogonal, the integral is small for \(n'_- \neq n_-\). Therefore the potentials \(V^{(\mathcal{N} - L)}_{n'_-;n'_+;n_-,n_+}(z)\) with \(n'_- \neq n_-\) only weakly couple the subsystems with different fixed \(n_-\) numbers.

A solution with fixed \(n_-\) may be called adiabatic approximation with respect to the electron motion, or “e-adiabatic approximation” for short. By analogy with the well known adiabatic approximation for electron motion in a strong magnetic field with a stationary Coulomb potential, it assumes that the Coulomb potential affects only the motion along the magnetic field, whereas the relatively fast motion in the transverse plane is governed...
functions (e.g., \(30\))

\[ g_{\kappa}(z) \sim \sin[\phi_{n_-,n_+,E}(z)] + \mathcal{R}_{E,\pm} \cos[\phi_{n_-,n_+,E}(z)], \]

(132)

where

\[ \phi_{n_-,n_+,E}(z) = k_\kappa z + \frac{m_+e^2}{\hbar^2 k_\kappa} \ln(k_\kappa z) \]

(133)

is the \(z\)-dependent part of the phase of the wave function at \(z \to +\infty\),

\[ k_\kappa = k_{n_-,n_+,E} = (2m_+E_\kappa)^{1/2}/\hbar \]

(134)

is the wavenumber, and \(E_\kappa\parallel = E - E_{n_-,n_+}[\text{Eq. (117)}].\)

D. Coupled channel formalism

In a strong magnetic field, the adiabatic approximation is a convenient starting point for solving the full system \(116\) by iterations, so that the leading longitudinal wave function in Eq. \(116\) remains the one corresponding to the starting adiabatic solution (cf. Ref. \(3\)). Then the numbering of the quantum states can be the same as in the adiabatic approximation, \(|\kappa\rangle = |N,L,n_-,n_{0+},\nu\rangle\) for the discrete spectrum and \(|\kappa\rangle = |N,L,n_-,n_{0+},E,\pm\rangle\) for the continuum. Here, \(n_-,n_{0+}\) are the values of \(n_-\) and \(n_+\) for the leading term in expansion \(114\).

1. Bound-state wave functions

For the bound states, the energies \(E_\kappa\) and \(E_\kappa\parallel\) are determined as the eigenenergies of the system of equations \(116\), and \(\nu = 0,1,2,\ldots\) corresponds to the longitudinal degree of freedom and controls the parity of the wave function. For the continuum, the energy \(E\) and the parity (\(\pm\)) are fixed arbitrarily. Since \(\hat{N}\) and \(L\) enter Eq. \(116\) only in combination \((N - L)\), the “longitudinal wave functions” \(g_{n_-,n_+;\nu}(z)\) can be numbered as \(g_{n_-,n_+;N,E,\pm}(z)\) for the discrete spectrum and \(g_{n_-,n_+;N,E,\pm}(z)\) for the continuum.

The degeneracy in \(N\), at a fixed \(N\), reflects the translational invariance. Indeed, different \(N\) correspond to different mean values of the squared total pseudomomentum projection on the \((xy)\)-plane, \(\langle \mathbf{r}_{\text{tot}},\perp^2 \rangle\), which according to Eqs. \(18\) and \(4\) is proportional to the squared sum of the guiding centers, \((\mathbf{r}_{c_-} + \mathbf{r}_{c_+})^2\), measured from the chosen gauge axis, which can be freely changed by the gauge transformation \(\mathbf{A}(\mathbf{r}) \to (1/2)\mathbf{B} \times (\mathbf{r} - \mathbf{r}_A)\) with arbitrary \(\mathbf{r}_A\) (cf. Ref. \(5\)).

Accordingly, for the physical problems that do not involve explicit positions of the guiding centers in space, including the present case of a single ion in a uniform field, one can identify the ion states by four quantum numbers instead of five: \(|\kappa\rangle = |N,n_-,n_{0+},\nu\rangle\).
2. Continuum wave functions

For the continuum, we construct the basis by analogy with the $R$-matrix formalism. Let $I_o$ be the total number of open channels at given $E$, i.e., number of such pairs $n_-, n_+$ that $E_{n_-, n_+} > E$. In this case, numbers $n_o \pm$ mark a selected open channel, defined for $E > E_{n_0-, n_0+}^\perp$ by asymptotic conditions at $z \to +\infty$

$$g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}(z) \sim C_{\text{norm}} \left\{ \delta_{n_o^-, n_{-o}} \delta_{n_o^+, n_{+o}} \sin[\phi_{n_o^-, n_o^+}; \kappa(z)] + \mathcal{R}_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm} \cos[\phi_{n_o^-, n_o^+}; \kappa(z)] \right\}, \quad (135)$$

where $z_{\text{max}}$ is half the normalization length, then the orthonormality of the transverse basis [$\text{Eq. (109)}$] leads to the condition

$$\sum_{n_-, n_+} \int_{-z_{\text{max}}}^{z_{\text{max}}} |g_{n_, n_+; \kappa}(z)|^2 dz = 1. \quad (137)$$

In the adiabatic approximation, a single term of the sum is retained in Eq. (137) for each open channel.

One can compose the basis of outgoing waves, appropriate to photoionization, by analogy with the case of the H atom in Refs. [31, 32]. The basis of outgoing waves with definite $z$-parity is defined by the asymptotic conditions at $z \to \infty$,

$$g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}(z) = 2i \sum_{n_{-}, n_{+}} \left[ (1 + i \mathcal{R}_{N, E, \pm})^{-1} \right]_{n_-, n_+; n_{-o}, n_{+o}+N, E, \pm} g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}(z). \quad (139)$$

Here, pairs $(n_-, n_+)$ and $(n', n'_+)$ run over open channels, but $(n_o^-, n_o^+)$ run over all (open and closed) channels. As follows from the orthonormality of the transverse basis, the normalization integral on the left-hand side of Eq. (136) equals

$$2z_{\text{max}} |C_{\text{norm}}|^2 \left[ 1 + \mathcal{S}_{N, E, \pm} \mathcal{S}_{N, E, \pm}^\dagger \right] = 4z_{\text{max}} |C_{\text{norm}}|^2, \quad (140)$$

where we have used the unitarity of the S-matrix. Then according to Eq. (136)

$$|C_{\text{norm}}| = (4z_{\text{max}})^{-1/2}. \quad (141)$$

After the orthonormal basis of outgoing waves have been obtained at given $N$ and $E$ for each $z$-parity, with $g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}(z) = \pm g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \mp}(z)$, we can easily construct solutions for electron waves propagating at $z \to \pm\infty$ in a definite open channel $(n_{0-}, n_{0+})$ for an arbitrary $L \leq N - n_-$. These solutions are given by Eq. (141) with coefficients

$$g_{n_o^-, n_o^+; \kappa}(z) = \frac{1}{\sqrt{2}} \left( g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, +}(z) \pm g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, -}(z) \right), \quad (142)$$

where the pairs $(n_o^-, n_o^+)$ relate to different open channels $(E > E_{n_o^-, n_o^+}^\perp)$, $\phi_{n_o^-, n_o^+}; E(z)$ is the $z$-dependent part of the phase of the wave function at $z \to +\infty$, defined in Eq. (133), and $C_{\text{norm}}$ is a normalization constant. The quantities $\mathcal{R}_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}$ with different pairs of $(n_o^-, n_o^+)$ and $(n_-, n_+)$, corresponding to the open channels, constitute the reactance matrix $\mathcal{R}_{N, E, \pm}$, which has dimensions $I_o \times I_o$. For the closed channels, defined by the inequality $E < E_{n_o^-, n_o^+}^\perp$, one should impose the boundary conditions $g_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}(z) \to 0$ at $z \to \infty$.

The set of solutions, defined by Eqs. (116) and (135), constitute a complete set of $I_o$ independent real basis functions. If the wave functions are normalized by the orthonormality of the transverse basis, the norm integral on the left-hand side of Eq. (136) equals

$$\int_{\mathbb{R}^2} dr_{+1} \int_{\mathbb{R}^2} dr_{-1} \int_{-z_{\text{max}}}^{z_{\text{max}}} dz |\psi_{\kappa}(r_{+1}, r_{-1}, z)|^2 = 1, \quad (136)$$

where $S_{n_o^-, n_o^+; n_{-o}, n_{+o}+N, E, \pm}$ are the elements of the unitary scattering matrix $S_{N, E, \pm} = (1 + i \mathcal{R}_{N, E, \pm})(1 - i \mathcal{R}_{N, E, \pm})^{-1}$.

The basis of outgoing waves is obtained from the real basis by transformation
where the sign $+$ or $-$ represents electron escape in the positive or negative $z$ direction, respectively. Waves incoming from $z \to \pm \infty$ are given by the complex conjugate of Eq. (142).

**E. Geometric sizes of the ions**

In order to evaluate populations of different bound levels and the collision frequency $\nu_{\text{coll}}$ in the plasma environment, it is useful to calculate the geometric sizes of the ions. For this aim we use the root-mean-square longitudinal and transverse sizes, $|\langle \kappa | z^2 | \kappa \rangle |^{1/2}$ and $|\langle \kappa | r^2 | \kappa \rangle |^{1/2}$, by analogy with Ref. [33]. Let us use the basis expansion (114) for calculation of these matrix elements. For the longitudinal mean squared size, using the orthonormality condition (109), we obtain

$$
\langle \kappa | z^2 | \kappa \rangle = \sum_{n_-, n_+} \int_{-z_{\text{max}}}^{z_{\text{max}}} g_{n_-, n_+; \kappa}(z) g_{n_-, n_+; \kappa}(z) z^2 \, dz.
$$

(143)

For the mean squared transverse size, using Eq. (80), we obtain

$$
\langle \kappa | r^2 | \kappa \rangle = 2 \langle \kappa | r_{+1} r_{-1} | \kappa \rangle = 2n_m^2 \langle \kappa | \hat{a}^\dagger \hat{a}^\dagger - \hat{a} \hat{a}^\dagger | \kappa \rangle.
$$

(144)

Then, using Eqs. (71a), (71b), (73a), and (73b), we obtain

$$
\langle \kappa | r^2 | \kappa \rangle = 2n_m^2 \sum_{n_- = 0}^\infty \sum_{n_+ = 0}^\infty \sum_{k = 0}^N \left( n_- + k + 1 \right) C_k^{(N, n_+)} C_k^{(N', n_+)} \int_{-z_{\text{max}}}^{z_{\text{max}}} g_{n_-, n_+; \kappa}(z) g_{n_-, n_+; \kappa}(z) \, dz
$$

$$
- \sum_{k = 0}^N \sqrt{(n_- + 1)(k + 1)} C_k^{(N, n_+)} C_k^{(N', n_+ + 1)} \int_{-z_{\text{max}}}^{z_{\text{max}}} g_{n_-, n_+ + 1; \kappa}(z) g_{n_-, n_+; \kappa}(z) \, dz
$$

$$
- \sum_{k = 0}^N \sqrt{n_- k} C_k^{(N, n_+)} C_k^{(N', n_+)} \int_{-z_{\text{max}}}^{z_{\text{max}}} g_{n_- - 1, n_+; \kappa}(z) g_{n_-, n_+; \kappa}(z) \, dz
$$

(145)

**V. INTERACTION WITH RADIATION**

**A. Radiative transitions**

In presence of an electromagnetic wave, its vector potential $A_{\text{rad}}$ should be added to the vector potential of the constant magnetic field $A$ in Eqs. (2) and (3). Then the total Hamiltonian of the system of an electron, a nucleus, a constant magnetic field, and radiation can be written as

$$
H_{\text{tot}} = \frac{1}{2m_+} \left( \mathbf{p}_+ - \frac{e}{c} A_{\text{rad}, \perp}(r_+) \right)^2
$$

$$
+ \frac{1}{2m_-} \left( \mathbf{p}_- + \frac{e}{c} A_{\text{rad}, \perp}(r_-) \right)^2
$$

$$
- \frac{Ze^2}{\sqrt{r^2 + z^2}} + \sum_{\mathbf{q}, \gamma} \hbar \omega_{\mathbf{q} \gamma} \hat{c}_{\mathbf{q} \gamma}^\dagger \hat{c}_{\mathbf{q} \gamma},
$$

(146)

where $\mathbf{q}$, $\alpha$, and $\omega_{\mathbf{q}}$ are the photon wavevector, polarization index, and frequency, respectively; $\hat{c}_{\mathbf{q} \gamma}$ and $\hat{c}_{\mathbf{q} \gamma}^\dagger$ are the photon creation and annihilation operators,

$$
A_{\text{rad}}(r) = \sum_{\mathbf{q}, \gamma} \left( \frac{2\pi \hbar c^2}{\omega_{\mathbf{q} \gamma} V} \right)^{1/2} \left( e_{\mathbf{q} \gamma} \hat{c}_{\mathbf{q} \gamma} e^{i \mathbf{q} \cdot \mathbf{r}} + e_{\mathbf{q} \gamma}^\dagger \hat{c}_{\mathbf{q} \gamma}^\dagger e^{-i \mathbf{q} \cdot \mathbf{r}} \right)
$$

(147)

is the electromagnetic field operator (in the Schrödinger representation), the subscripts $\perp$ and $z$ mark the transverse and longitudinal vector components with respect to the magnetic field direction, and $V$ is the normalization volume (see, e.g., Refs. [23, 38]).

The operator of interaction with radiation is obtained by expanding the brackets in Eq. (146). We will use the Coulomb gauge, $\nabla \cdot A_{\text{rad}} = 0$, and the transverse approximation assuming $\mathbf{q} \cdot e_{\mathbf{q} \gamma} = 0$. Then operator $A_{\text{rad}}$ commutes with $\pi_\pm$, so that $A_{\text{rad}} \cdot \pi_\pm + \pi_\pm \cdot A_{\text{rad}} = 2A_{\text{rad}} \cdot \pi_\pm$.

Neglecting nonlinear effects (i.e., terms proportional to $A_{\text{rad}}^2$), we obtain the following operator that couples internal degrees of freedom to radiation:

$$
V_{\text{int}} = \frac{e}{m_+ c} A_{\text{rad}, \perp}(r_-) \cdot \pi_- - \frac{Ze}{m_+ c} A_{\text{rad}, \perp}(r_+) \cdot \pi_+
$$

$$
+ \frac{e}{m_- c} A_{\text{rad}, z}(r_-) p_{-z} - \frac{Ze}{m_- c} A_{\text{rad}, z}(r_+) p_{+z}.
$$

(148)
Using Eq. (147), we can rewrite Eq. (148) as
\[
V_{\text{int}} = \sqrt{\frac{2e\hbar}{\gamma c}} \sum_{q} \left( c_{q} e_{q} \cdot j_{\text{eff}} + e_{q}^{*} j_{\text{eff}}^{\dagger} c_{q}^{\dagger} \right),
\] (149)
where
\[
j_{\text{eff}} = e^{iq \cdot \sigma} (e \hat{r}_{-} - Ze \hat{r}_{+})
\] (150)
is the effective current operator \((\hat{r}_{\pm} = \pi_{\pm}/m_{\pm})\).

Let us consider an absorption of a photon with a given wavevector \(q\) and polarization \(\alpha\). The initial state is \(|i\rangle = f_{q}(1)|\psi_{i}\rangle\) and the final state is \(|f\rangle = f_{q}(0)|\psi_{f}\rangle\), where \(|\psi_{i,f}\rangle\) denotes the state of the system of charged particles and \(f_{q}(N)\) is the function of photon number \(23\). According to the Fermi’s golden rule, probability of transition, per unit time, from initial quantum state \(f_{q}(1)|i\rangle\) to final state \(f_{q}(0)|f\rangle\) with absorption of one photon is given by
\[
d\omega_{i\rightarrow f} = \left( \frac{2\pi}{\hbar} \right) \left| \langle \psi_{f} | j_{\text{eff}}^{\dagger} | \psi_{i} \rangle \right|^{2} \delta(E_{f} - E_{i} - \hbar \omega_{q}) \, d\nu_{f},
\] (151)
where \(E_{i}, E_{f}\), and \(\hbar \omega_{q}\) are the energies of the initial state, final state, and absorbed photon, respectively, and \(d\nu_{f}\) is the density of final states. Taking into account the properties of the photon creation and annihilation operators \(23\), \(c_{q}^{\dagger} f_{q}(N) = \sqrt{N} f_{q}(N-1), c_{q}^{\dagger} f_{q}(N) = \sqrt{N+1} f_{q}(N+1)\), where \(f_{q}(N)\) is the function of photon number, and performing normalization of transition rate \(151\) by the photon flux \(c/\mathcal{V}\), we arrive at the differential cross section
\[
d\sigma_{i\rightarrow f, q\gamma} = \frac{4\pi^{2}}{\omega_{q} c} \left| \langle \psi_{f} | e_{q} \cdot j_{\text{eff}} | \psi_{i} \rangle \right|^{2} \delta(E_{f} - E_{i} - \hbar \omega_{q}) \, d\nu_{f}.
\] (152)

If the final state belongs to the discrete spectrum, the final energies \(E_{f}\) are distributed within a narrow band around the value \(E_{f0} = E_{i} + \hbar \omega_{f} i\), where \(\omega_{f} i\) is a central value of the transition frequency. Then integration of Eq. (152) over the final states gives
\[
\sigma_{i\rightarrow f, q\gamma} = \frac{4\pi^{2}}{\hbar \omega_{q} c} \left| \langle \psi_{f} | e_{q} \cdot j_{\text{eff}} | \psi_{i} \rangle \right|^{2} \Delta_{f_{1}}(\omega_{q} - \omega_{f_{1}}),
\] (153)
where \(\Delta_{f_{1}}(\omega_{q} - \omega_{f_{1}})\) describes the profile of the spectral line, which is normalized so that \(\int \Delta_{f_{1}}(\omega) \, d\omega = 1\).

If the final state belongs to the continuum and wave functions are normalized according to Eq. (150), then
\[
d\nu_{f} = \frac{\pi}{\hbar^{2} k_{f}} \, dE_{f},
\] (154)
\[
k_{f} = \frac{\hbar^{-1}}{\sqrt{2m_{*} E_{f}^{\|}}}, \quad E_{f}^{\|} \equiv E_{f} - E_{n_{-1},0,n_{0}+1}^{\perp},
\] (155)
with \(E_{f} - E_{n_{-1},0,n_{0}+1}^{\perp} > 0\). In this case the cross section of photoabsorption takes the form
\[
\sigma_{i\rightarrow f, q\gamma} = \frac{4\pi \omega_{q}}{\hbar^{2} k_{f} \omega_{q} c} \left| \langle \psi_{f} | e_{q} \cdot j_{\text{eff}} | \psi_{i} \rangle \right|^{2}.
\] (156)

The above equations do not include the photon interaction with magnetic moments \(\hat{\mu}_{\pm}\) of the particles. For transitions without spin-flip, the latter interaction can be taken into account by supplementing the operator \(e_{q} \cdot j_{\text{eff}}\) by the term \(-i(q \times e) \cdot (\hat{\mu}_{-} + \hat{\mu}_{+})\) (cf. 35), whereas operators \((q \times e) \times \hat{\mu}_{\pm}\) are responsible for spin-flip transitions (cf. 36). The corresponding contributions to the transition matrix elements are proportional to \(q\) and prove to be of the same order of magnitude as the first-order corrections \((\propto q)\) to the dipole approximation that we use below. Therefore, these terms will be neglected in the dipole approximation.

### B. Dipole approximation

In the dipole approximation for the matrix elements of radiative transitions, \(e^{iq \cdot \sigma}\) is replaced by 1. For bound-bound and bound-free transitions this is justified, provided that the mean bound-state size \(l\) is much smaller than \(q^{-1} = \omega_{q}/c\). Since the binding energy \(E_{b}\) is by the order of magnitude \(\sim Ze^{2}/l\), this requirement translates into \(\hbar \omega_{q} \ll \alpha_{l}^{-1} E_{b}/Z\), where \(\alpha_{l} = c^{2}/\hbar c\) is the fine structure constant. In this approximation, the effective current \(150\) takes the form
\[
j_{\text{eff}} = \frac{e}{m_{\pm}} \pi_{-} - \frac{Ze}{m_{\pm}} \pi_{+}.
\] (157)

Using the commutation relation
\[
[\pi_{\pm}, H_{0}] = i \hbar [H_{0}, r_{\pm}],
\] (158)
where \(H_{0}\) is the field-free Hamiltonian given by Eq. (34), we can transform “velocity form” of the matrix element in Eq. (152) to the “length form” (cf., e.g., Ref. 37)
\[
\langle \psi_{f} | j_{\text{eff}} | \psi_{i} \rangle = -i \hbar^{-1} (E_{f} - E_{i}) D_{f_{1}} = i \omega_{c} D_{f_{1}}.
\] (159)

Here, \(D_{f_{1}} = \langle \psi_{f} | D | \psi_{i} \rangle\) is the matrix element of the electric dipole moment,
\[
D = Ze r_{+} - e r_{-} = (Z - 1)e R - e r.
\] (160)

For the bound-bound transitions, substitution of Eq. (159) into Eq. (153) gives
\[
\sigma_{i\rightarrow f, q\gamma} = \frac{4\pi^{2} \omega_{q}}{\hbar^{2} c} |e_{q,\gamma} \cdot D_{f_{1}}|^{2} \Delta_{f_{1}}(\omega_{q} - \omega_{f_{1}}).
\] (161)

For the bound-free transitions, substitution of Eq. (159) into Eq. (156) gives
\[
\sigma_{i\rightarrow f, q\gamma} = 4\pi \omega_{q} \frac{m_{*} \omega_{q}}{\hbar^{2} k_{f} c} |e_{q,\gamma} \cdot D_{f_{1}}|^{2}.
\] (162)

In the cyclic coordinates \(34\), we have
\[
e_{q,\gamma} \cdot D_{f_{1}} = \sum_{\alpha=-1}^{1} e_{q,\gamma,-\alpha} D_{f_{1},\alpha}.
\] (163)
Using Eq. (80), we can write the transverse (right and left) cyclic components of the dipole operator $D$ as

$$
D_{+1} = (Z - 1)e a_{m, Z - 1}(\hat{b} - \hat{b}^\dagger) - e a_m(\hat{a}^\dagger - \hat{a}) = e a_m[\sqrt{Z - 1}(\hat{b} - \hat{b}^\dagger) - \hat{a}^\dagger + \hat{a}],
$$

$$
D_{-1} = (Z - 1)e a_{m, Z - 1}(\hat{b} - \hat{b}^\dagger) - e a_m(\hat{a} - \hat{a}^\dagger) = e a_m[\sqrt{Z - 1}(\hat{b}^\dagger - \hat{b}) - \hat{a} + \hat{a}^\dagger],
$$

whereas the longitudinal component $D_0 = -e \mathbf{z}$ does not affect the transverse states of motion. From these equations and Eqs. (71), (73), and (82) we see that $D_\alpha$ transforms each pure transverse state $|N, \tilde{N}, n, \tilde{n}\rangle$ into the superposition of such states,

$$
D_{+1} |N, \tilde{N}, n, \tilde{n}\rangle = e a_m \sqrt{Z - 1} \left[ \sqrt{N} |N - 1, \tilde{N} - 1\rangle_1 - \sqrt{N + 1} |N, \tilde{N} + 1\rangle_1 \right] \otimes |n, \tilde{n}\rangle_2
- e a_m |N, \tilde{N}\rangle_1 \otimes \left[ \sqrt{n + 1} |n + 1, \tilde{n}\rangle_2 - \sqrt{n} |n, \tilde{n} - 1\rangle_2 \right],
$$

$$
D_{-1} |N, \tilde{N}, n, \tilde{n}\rangle = e a_m \sqrt{Z - 1} \left[ \sqrt{N + 1} |N + 1, \tilde{N}\rangle_1 - \sqrt{N} |N, \tilde{N} - 1\rangle_1 \right] \otimes |n, \tilde{n}\rangle_2
- e a_m |N, \tilde{N}\rangle_1 \otimes \left[ \sqrt{n} |n - 1, \tilde{n}\rangle_2 - \sqrt{n + 1} |n, \tilde{n} + 1\rangle_2 \right].
$$

It follows that $D_\alpha$ transforms a state with a definite $L = \tilde{N} - N + n - \tilde{n}$ into a state with $L' = L + \alpha$. This entails the selection rule

$$
L_f = L_i + \alpha.
$$

It reflects conservation of the total angular momentum of the entire system, comprising an electron, a nucleus, and a photon. As a consequence, in the right-hand side of Eq. (162) we can use the expansion

$$
|e_{q\gamma} \cdot D_{f,j}|^2 = \sum_{\alpha = -1}^{1} |e_{q\gamma, -\alpha}|^2 |D_{f,i,\alpha}|^2.
$$

Terms $e_{-\alpha} e_{\alpha}' D_{f,i,\alpha} D_{f,i,\alpha}'$ with $\alpha \neq \alpha'$ are absent, because $D_\alpha$ and $D_{\alpha'}$ transform a pure quantum state $|\psi_i\rangle$ into states $|\psi_f\rangle$ and $|\psi_f'\rangle$ with different $z$-projections of the angular momentum, so that $D_{f,i,\alpha}$ and $D_{f,i,\alpha'}$ cannot be non-zero simultaneously. Thus Eqs. (161) and (162) can be written as

$$
\sigma_{i \rightarrow f, q\gamma} = \sum_{\alpha = -1}^{1} |e_{q\gamma, \alpha}|^2 \sigma_{i \rightarrow f, \alpha}^{(\mathbf{b}, \mathbf{f})} (\omega_q)
$$

where

$$
\sigma_{i \rightarrow f, \alpha}^{(\mathbf{b})} (\omega) = \frac{4\pi^2 \omega}{\hbar c} |D_{f,i,\alpha}|^2 \Delta_{f,i} (\omega - \omega_{f,i}),
$$

$$
\sigma_{i \rightarrow f, \alpha}^{(\mathbf{f})} (\omega) = 4z_{\max} \frac{\pi m_o \omega}{\hbar c e k_f} |D_{f,i,\alpha}|^2
$$

for the bound-bound and bound-free transitions, respectively.

Neglecting the Doppler broadening, we can model $\Delta_{f,i} (\omega)$ in Eq. (174) by the Lorentz-Cauchy profile,

$$
\Delta_{f,i} (\omega) = \frac{1}{\pi} \frac{\nu_{\text{eff}}}{(\omega - \omega_{f,i})^2 + \nu_{\text{eff}}^2},
$$

where $\nu_{\text{eff}}$ is an effective damping frequency. In the simplest approximation, $\nu_{\text{eff}} = \nu_{\text{coll}} + \nu_{\text{rad}}$, where $\nu_{\text{coll}}$ is an effective frequency of collisions of a given ion with plasma particles, and

$$
\nu_{\text{rad}} = \frac{4\omega_{fi}^3}{3\hbar c^2} \sum_{\alpha = -1}^{1} |D_{f,i,\alpha}|^2
$$

is the natural radiative width (cf., e.g., [35]).

For practical computations, it is convenient to consider the continuum wave functions normalized so that the amplitude of the outgoing wave in a selected open channel equals 1 at infinity. Then the factor $4z_{\max}$ in Eq. (172) drops out from the numerical code, being canceled by the squared normalization constant (141).

Kopidakis et al. [35] defined a dimensionless interaction operator, which can be written as

$$
\hat{M} = \frac{2\hbar}{e \omega} e_{q\gamma} \cdot \mathbf{J}_{\text{eff}}.
$$

The correspondence between the “velocity form” and “length form” of this operator has been discussed in Ref. [31] regarding the problem of a hydrogen atom in a strong magnetic field. It was also employed in Ref. [32] for treatment of the bound-free transitions of a hydrogen atom moving in the magnetic field. Using the dipole approximation, we can rewrite Eq. (172) in the same form as Eq. (7) of [32],

$$
\sigma_{i \rightarrow f, \alpha}^{(\mathbf{f})} (\omega) = \frac{\pi \alpha (z_{\max})}{k_f} \frac{\hbar a}{\hbar \omega} m_o |M_{f,i,\alpha}|^2
= 2\pi \alpha \frac{\hbar c e k_f}{\hbar \omega} \sqrt{\frac{\hbar c e k_f}{\hbar \omega}} m_o Z_{\max} a_B |M_{f,i,\alpha}|^2,
$$

where $M_{f,i,\alpha} = i(\hbar / \omega) D_{f,i,\alpha} / e a_B$ is the respective cyclic component of the dimensionless matrix element.
\[ \langle \psi_f | e_{q,2} \cdot \hat{M} | \psi_i \rangle, \quad a_B = \hbar^2/m_e e^2 \] is the Bohr radius, \( H_a = 2\text{Ry} = e^2/\alpha \text{B} \) is the Hartree energy unit, \( \alpha \) being the Rydberg energy and \( m_e \) the electron mass.

For the bound-bound transitions, it is customary to define dimensionless oscillator strengths (e.g., [19])

\[ f_{\alpha} = \frac{\hbar \omega}{\text{Ry}} \left| \frac{D_{\alpha}}{a_B} \right|^2. \] (177)

In these notations, Eq. (171) can be written as

\[ \sigma_{\alpha}^{\text{bb}}(\omega) = 2\pi^2 e^2 m_e c f_{\alpha} \Delta f_{\alpha}(\omega). \] (178)

C. Expansion on the transverse basis

Let us use the basis expansion (114) for calculation of the matrix elements \( D_{f,\alpha} = \langle \psi_f | D_{\alpha} | \psi_i \rangle \). For the longitudinal polarization (\( \alpha = 0 \)), using the orthonormalization condition (100), we obtain

\[ D_{f,0,0} = -e\delta_{N_f,N_i} \delta_{L_f,L_i} \sum_{n_-,n_+} g_{n_-,n_+}^* g_{n_-,n_+}(\kappa,\zeta) \int dz. \] (179)

In the adiabatic approximation, we are left with the only term with \( n_- = n_- i = n_-, f \) and \( n_+ = n_+ i = n_+, f \), while transitions with \( n_- \neq n_- f \) or \( n_+ \neq n_+, f \) are forbidden. Beyond the adiabatic approximation, the latter transitions are allowed, but \( |D_{f,0,0}| \) is small compared to the case without changing \( n_- \) and \( n_+ \). For the initial and final states with definite \( z \)-symmetry, the corresponding selection rule follows: \( D_{f,0} \) is non-zero only for transitions between the state of opposite \( z \)-symmetry. In particular, bound-bound transitions between states with \( \nu_i \) and \( \nu_f \) of the same parity (both even or both odd) are dipole forbidden.

For the circular polarizations \( \alpha = \pm 1 \), using Eq. (52), we can transform Eqs. (174) and (175) to

\[ \frac{D_{+1}}{ea_m} = \frac{i a_m}{\hbar} U^\dagger \pi^+ \pi \hat{N} \hat{\alpha} \hat{N} \hat{\alpha} U - \hat{a} \hat{a} - \sqrt{\hat{N} - 1} \hat{b} \hat{b}, \] (180)

\[ \frac{D_{-1}}{ea_m} = -\frac{i a_m}{\hbar} U^\dagger \pi^- \pi \hat{N} \hat{\alpha} \hat{N} \hat{\alpha} U - \hat{a} \hat{a} - \sqrt{\hat{N} - 1} \hat{b} \hat{b}. \] (181)

The first term in each of these equations shifts the quantum number \( n_+ \) by \( \pm 1 \) according to Eq. (51), the second term shifts the number \( n_- \) according to Eqs. (71c), (71d), (73d), and (73b), while the last term shifts the number \( \hat{N} \) according to Eqs. (71c), (71d), (73a), and (73d). In all cases the selection rule (108) holds. Thus the transverse basis states (101) are transformed as

\[ D_{f,0,0} = \sqrt{Z} \sqrt{n_+} \hat{N} \hat{\alpha} \hat{N} \hat{\alpha} \hat{a} \hat{a} - \sqrt{\hat{N} + 1} \hat{a} \hat{a} - \sqrt{\hat{N} - 1} \hat{b} \hat{b}. \] (182)

Let us substitute the basis expansion (102) into \( D_{f,0} \) with \( \alpha = \pm 1 \) and use relations (182) and (183). Then for transitions with \( L_f = L_i \pm 1 \) and \( \hat{N}_f = \hat{N}_i \), taking into account the orthogonality relation (109), we obtain

\[ \frac{D_{f,0,0}}{ea_m} = \sqrt{Z} \sum_{n_+ = 0}^{N} \sqrt{n_+} \sum_{n_- = 0}^{\infty} \mathcal{L}_{n_-,n_+} (\kappa,\kappa') |\kappa_i\rangle - \sum_{n_+ = 0}^{N} \sqrt{n_+ + 1} \sum_{n_- = 0}^{\infty} \mathcal{L}_{n_-,n_+} (\kappa,\kappa') |\kappa_i\rangle, \] (184)

\[ \frac{D_{f,0,0}}{ea_m} = \sqrt{Z} \sum_{n_+ = 0}^{N} \sqrt{n_+ + 1} \sum_{n_- = 0}^{\infty} \mathcal{L}_{n_-,n_+} (\kappa,\kappa') |\kappa_i\rangle. \] (185)

where \( \mathcal{N} \equiv \hat{N}_i - L_i + n_- \) and \( \mathcal{L} \) denotes the longitudinal overlap integral,

\[ \mathcal{L}_{n_-,n_+} (\kappa',\kappa) = \int_{-\pi/2}^{\pi/2} g_{n_-,n_+}^* \kappa' g_{n_-,n_+} \kappa \, dz. \] (186)

The last term in each of equations (182) and (183) corresponds to transitions with \( L_f = L_i + \alpha \) and \( \hat{N}_f = \hat{N}_i + \alpha \), which leave \( \hat{N} - L \) un-changed. The corresponding dipole matrix elements equal \( ea_m \sqrt{(Z-1)\text{max}(\mathcal{N}_i,\mathcal{N}_f)} |\psi_i\rangle |\psi_f\rangle = 0 \), because \( \psi_i \) and \( \psi_f \) are orthogonal. The absence of such transitions agrees with the degeneracy of the problem in \( \hat{N} \), discussed above. Thus it is sufficient to study only the transitions between states with \( \hat{N} = 0 \); the results for non-zero \( \hat{N} \) are then obtained by adding \( \hat{N} \) to both \( L_i \) and \( L_f \).
VI. APPROXIMATE SOLUTIONS FOR ULTRA-STRONG FIELDS

In this section we consider an approximate treatment of the hydrogenlike ion in the full adiabatic approximation (Sect. VI C), using the method previously developed by Hasegawa & Howard [19], for a strongly magnetized H atom.

A. Wave functions and eigenenergies

Let us find an approximate solution to the Schrödinger equation in the adiabatic approximation, Eq. (130), for the bound states. Following Hasegawa & Howard [19], we find asymptotic solutions at small and large z and match them at an intermediate point

\[ z_0 = C a_m^\lambda, \quad 0 < \lambda < 2/3, \]  

(187)

where C and \( \lambda \) are constants, independent of \( z \) and \( a_m \). The matching is provided by equating the logarithmic derivatives

\[ \eta(z) = \frac{g'_k(z)}{g_k(z)} \]  

(188)

of the interior and exterior solutions at \( z = z_0 \). The bounds on \( \lambda \) in Eq. (187) ensure that \( z/a_m \to \infty \) and \( z^2 |\ln a_m| \to 0 \) with \( a_m \to 0 \) for all \( z > z_0 \), which is needed for validation of the approximate exterior solution (Sect. VI A 1), while \( z^2/a_m \to 0 \) for all \( z < z_0 \), as required for the validity of the approximate exterior solution (Sect. VI A 2).

1. Exterior solution for bound states

At \( \zeta \to \infty \) all effective potentials \( V_{0,n+}^{(N)}(z) \) converge to the 1D Coulomb potential, so that Eq. (130) is replaced by

\[ -\frac{\hbar^2}{2m_e} \frac{d^2 g_k}{dz^2} - \frac{Ze^2}{|z|} g_k = E_\parallel g_k. \]  

(189)

The well known solution to this equation for a bound state (i.e., for \( E_\parallel < 0 \), so that \( \lim_{z \to \infty} g_k(z) = 0 \)) is

\[ g_{\text{ext}}(z) = C W_{\nu,\frac{\lambda}{2}}(2z/\tilde{\nu}a_s), \]  

(190)

where \( W_{\nu,\frac{\lambda}{2}}(x) \) is the Whittaker function [22], \( C \) is a normalization constant,

\[ a_s = \frac{\hbar^2}{m_e Ze^2}, \]  

(191)

is the “effective Bohr radius”, \( \tilde{\nu} \) is the “effective principal quantum number” defined through the relation

\[ \epsilon_\kappa = \frac{E_\parallel}{Ry_*} = \frac{1}{\tilde{\nu}^2}, \]  

(192)

where

\[ Ry_* = \frac{Z^2 e^4 m_*}{2\hbar^2} = \frac{Z^2 m_*}{m_e} \]  

(193)

is the “effective Rydberg energy”.

At small (but non-zero) argument \( x = 2z/\tilde{\nu}a_s \) and non-integer \( \tilde{\nu} \), the Whittaker function can be expanded as [19]

\[ W_{\nu,\frac{\lambda}{2}}(x) = -\Gamma(\tilde{\nu})\left[\tilde{\nu}x - (\tilde{\nu}x)^2\right] \cos \tilde{\nu} \pi \]  

\[ + \left[ -1 + \tilde{\nu} x \left( \ln x - \frac{1}{2} \frac{1}{\tilde{\nu}^2} + \psi(\tilde{\nu}) - \psi(1) - \psi(2) \right) \right] \frac{\sin \tilde{\nu} \pi}{\pi} \]  

\[ + O(\tilde{\nu} x \ln x), \]  

(194)

where

\[ \psi(x) = \frac{d \ln \Gamma(x)}{dx} \]  

(195)

is the digamma function [22]: \( \psi(1) = \psi(2) - 1 = -\gamma_E \), where \( \gamma_E = 0.5772\ldots \) is the Euler-Mascheroni constant.

If \( z_0 \) were zero, \( \tilde{\nu} \) would be an integer. At non-zero \( z_0 \), with \( a_m \to 0 \), \( \tilde{\nu} \) tends to integer values in such a way that \( \sin \tilde{\nu} \pi \) tends to zero logarithmically (as will be seen from the solutions below), that is slower than \( z_0 \to 0 \). Therefore, \( z_0 \cos \tilde{\nu} x \to 0 \), and from Eq. (194) we obtain

\[ W_{\nu,\frac{\lambda}{2}}(2z_0/\tilde{\nu}a_s) = \Gamma(\tilde{\nu}) \frac{\sin \tilde{\nu} \pi}{\pi} \left[ 1 + O\left( a_m^{-\lambda} \cot \tilde{\nu} \pi \right) \right]. \]  

(196)

Taking the derivative in Eq. (194) and dividing by \( \tilde{\nu} \), we obtain the logarithmic derivative in the form

\[ \eta_{\text{ext}} = \frac{d}{dz} \ln W_{\nu,\frac{\lambda}{2}}(2z/\tilde{\nu}a_s) \approx -2 \frac{2}{a_s} \left( \ln \frac{2 z}{a_s} + \pi \cot \tilde{\nu} \pi + 2 \gamma_E - \Theta(\tilde{\nu}) \right), \]  

(197)

where \( z \sim z_0 \ll a_s \) and

\[ \Theta(\tilde{\nu}) = \ln \tilde{\nu} - \frac{1}{2\tilde{\nu}^2} - \psi(\tilde{\nu}) = \ln \tilde{\nu} + \frac{1}{2\tilde{\nu}^2} - \psi(1 + \tilde{\nu}). \]  

(198)

2. Interior solution for even states

Now let us consider \( |z| \ll z_0 \). In terms of the dimensionless coordinate \( \zeta [120] \), the Schrödinger equation in the adiabatic approximation [Eq. (130)] becomes

\[ \frac{d^2 g_\kappa}{d\zeta^2} + \frac{3/2 a_m}{a_s} V_{0,n+}^{(N)}(\zeta) g_\kappa - 2 \left( \frac{a_m}{a_s} \right)^2 e_\kappa g_\kappa = 0, \]  

(199)

where \( e_\kappa \) is the dimensionless eigenvalue defined in Eq. (192). We solve this equation approximately, using the perturbation theory with respect to the small
FIG. 2: Dependence of the quantities $J_{Nn}$ [Eq. (203)] on quantum number $N$ (left panel, for $n_+ = 0, 1, 2, 3,$ and 4) and on quantum number $n_+$ (right panel, for $N$ from 0 to 20) for $Z = 2$ (dots connected by solid lines) and $Z = 6$ (triangles connected by dashed lines).

parameter $a_m/a_*$ separately for the even and odd states. Since in this section we are interested in the bound states, $E_n^0 < 0$, we can safely set $n_- = 0$. Then $N = \tilde{N} - L$ and

$$v_{0,n_+}^{(N)} = \sum_{k=0}^{N} \left(C_k^{(N,n_+)}\right)^2 \int_0^\infty \frac{I_{k,0}(\rho)}{\sqrt{\rho + \zeta^2}} \, d\rho,$$

(200)

where, according to Eq. (25), $I_{k,0}(\rho) = \rho^{k/2}e^{-\rho/2}/k!$, and coefficients $C_k^{(N,n_+)}$ are given by the relation (112) and normalization (113).

Let us consider even states. In the first approximation (linear in $a_m/a_*$), the last term in Eq. (199) drops out, and the solution is proportional to

$$1 - \frac{2^{3/2}a_m}{a_*} \int_0^\zeta d\zeta' \int_0^{\zeta''} v_{0,n_+}^{(N)}(\zeta'') \nu_{int}(z) \approx -\eta_{int}(z) = -\frac{2}{a_*} \int_0^{2^{3/2}a_m/\sqrt{\pi}} d\zeta v_{0,n_+}^{(N)}(\zeta) \approx -\frac{2}{a_*} \int_0^{2^{3/2}a_m/\sqrt{\pi}} d\zeta v_{0,n_+}^{(N)}(\zeta).$$

(201)

The logarithmic derivative for the interior solution becomes

$$\eta_{int}(z) = -\frac{1}{a_*} \left[ 2 \ln \frac{z_0}{a_m} + \ln 2 + \gamma_E - J_{Nn_+} + O \left( \frac{a_m^2}{z_0^2} \right) \right],$$

(202)

where $H_k = \sum_{n=1}^{k} n^{-1}$ is the $k$th harmonic number, $J_{00} = 0$, and for $N \geq 1$

$$J_{Nn_+} = \sum_{k=1}^{N} H_k \left(C_k^{(N,n_+)}\right)^2.$$

(203)

In the particular case $N = 0$, which corresponds to the non-moving ion, Eq. (202) reduces to the result of Hasegawa & Howard [19]. For $N = 1$, we obtain

$$J_{10} = \frac{Z - 1}{Z}, \quad J_{11} = \frac{1}{Z}.$$

(204)

The dependence of the quantities $J_{Nn_+}$ on the quantum numbers $N$ and $n_+$ is shown in Fig. 2.

3. Binding energies of even states

By equating $\eta_{int}$ (202) to $\eta_{ext}$ (197) at $z = z_0$ we obtain the following equation for the effective quantum number $\tilde{\nu}$:

$$\pi \cot \tilde{\nu} + \Theta(\tilde{\nu}) = \ln \frac{a_*}{2a_m} + \frac{\ln 2 - 3\gamma_E - J_{Nn_+}}{2}$$

(205)

($|\sin \tilde{\nu} - 1| \ll 1$), where $\Theta(\tilde{\nu})$ is defined by Eq. (118). Solution of Eq. (205) gives the longitudinal energies of the even states through Eq. (112).

The lowest-energy state for each $N$ and $n_+$ (so called tightly bound state) corresponds to $\tilde{\nu} \ll 1$. In this case,
the series expansion (22, 6.3.14, 23.2), \( \psi(1 + \tilde{v}) = -\gamma_E + (\pi^2/6)\tilde{v} - (\pi^4/90)\tilde{v}^2 + \ldots \) leads to an approximate relation \( \Theta(\tilde{v}) \approx \ln \tilde{v} + 1/(2\tilde{v}) + \gamma_E - (\pi^2/6)\tilde{v} \). To the same accuracy up to \( O(\tilde{v}^2) \), \( \pi \cot \pi \tilde{v} \approx \tilde{v}^{-1} - \pi^2/3 \). Thus from Eq. (206) we get approximately
\[
\frac{1}{\tilde{v}} = \ln \frac{\gamma_*}{2} + 2\ln \tilde{v} - \gamma_E - J_{Nn_+} + \frac{\pi^2}{3}\tilde{v},
\]
where we have introduced the magnetic-field parameter
\[
\gamma_* = \frac{a_i^2}{a_m^2} = \frac{h^3B}{Z^2m_e^3c^3} = \frac{B}{B_*},
\]
which should be large in the considered approximation. Here, \( B_* \equiv Z^2m_e^2e^3c/h^3 \approx 2.35 \times 10^9 (m_e/m_e)^2Z^2 \) G. 
Equation (206) can be easily solved numerically. For example, as long as \( \ln(\gamma_* / 2) > \gamma_E + J_{Nn_+} \), one can use iterations of the form
\[
\tilde{v}_{i+1} = w \left( \ln \frac{\gamma_*}{2} + 2\ln \tilde{v}_i - \gamma_E - J_{Nn_+} + \frac{\pi^2}{3}\tilde{v}_i \right)^{-1}
+ (1 - w) \tilde{v}_i
\]
with an appropriate weight \( w \), starting from
\[
\frac{1}{\tilde{v}_0} = \ln \frac{\gamma_*}{2} - \gamma_E - J_{Nn_+}.
\]

Having tried different values of \( w \) at different \( \gamma_* \) we found that a good choice of \( w \), which provides a quick convergence of the iterations, can be roughly approximated as \( w = (1 + 4\tilde{v}_0^{3/2})/(1 + 15\tilde{v}_0^{3/2}) \).

In the ground state, \( N = n_+ = 0 \), and Eq. (206) without the last (linear in \( \tilde{v} \)) term reproduces the result of Hasegawa and Howard [19]. However, by means of a comparison with the numerical results from Ref. [16] we found that even at the superstrong field strengths \( B \sim 10^{15} \) G, encountered in magnetars, a solution of such a truncated equation produces an unacceptable error \( \sim 200 \) eV in the ground-state energy. The linear term in Eq. (206) considerably improves the accuracy.

In Fig. 3 we show the dependence of energy \( E_n = E_{n_0} + \hbar \omega_{n_+} \) on the magnetic field strength \( B \) and on the quantum number \( N \) (the left and right panels, respectively). The “electron cyclotron” quantum number \( n_- \) must equal zero in the displayed energy range. The zero-point energy \( E_{n_0} \) is dismissed, because it does not affect the binding, being the same for the bound and unbound states. It is of interest to compare the \( B \)-dependences of our analytic estimates of energy shown in the left panel with Fig. 2 in Ref. [16], which shows the analogous dependences computed numerically. We can notice a qualitative difference at \( B < 10^{14} \) G, where different energy branches overlap in our figure. This difference is caused
by the fact that our analytic estimates have a good accuracy only at superstrong fields. At such high fields, however, the branches corresponding to non-zero \( n_+ \) merge into continuum, because \( E_n^{||} \) increases slower (logarithmically) than the energy of transverse excitations \( n_- \hbar \omega_{c+} \). Ultimately, at \( B \gtrsim 7 \times 10^{14} \) G only the branch with \( n_+ = 0 \) survives, while the states with \( n_+ > 0 \) become metastable (i.e., turn into continuum resonances).

The case where \( \nu \) is not small corresponds to the “loosely-bound” or “hydrogenlike” states. As long as the logarithm on the right-hand side of Eq. (205) is large, this equation can be satisfied only if \( \cot \tilde{\nu} \pi \) is also large (tends to infinity at \( a_m \to 0 \)). Then we can write

\[
\tilde{\nu} = \frac{\nu_\parallel}{2} + \delta_{\nu_\parallel}, \quad \nu_\parallel = 2, 4, 6, \ldots ,
\]

(210)

where the even numbers \( \nu_\parallel \) enumerate the even states and the quantum defect \( \delta_{\nu_\parallel} \) is given by

\[
\frac{1}{\delta_{\nu_\parallel}} \approx \pi \cot \pi \delta_{\nu_\parallel} \approx \frac{1}{2} \left( \ln \frac{\gamma_\parallel}{2} - 3\gamma_E - J_{Nn_+} \right) + \Theta \left( \frac{\nu_\parallel}{2} \right)
\]

(211)

where \( \Theta \) is defined by Eq. (198).

The “tightly-bound” solution described above [Eq. (206)] corresponds formally to \( \nu_\parallel = 0 \). One should note that the approximations (206) and (211) are based on the condition that the right-hand side in Eq. (205) is large, implying that \( J_{Nn_+} \ll \ln \gamma_\parallel \). One can show (see Appendix C) that \( J_{N0} \sim \ln \gamma_\parallel \cdot \gamma_\parallel \gg 1 \). Therefore, the necessary condition of the applicability of the approximations (206) and (211) for the states with \( n_+ = 0 \) is \( \ln(\gamma_\parallel/N) \gg 1 \). If this is not the case, one has to use Eq. (205) instead of the approximations (206) or (211).

4. Odd bound states

For the odd-parity states, the longitudinal wave function \( g_n(z) \) tends to zero at \( z \to 0 \). Therefore it is small in the region \( |z| \lesssim a_m \), where the effective potentials \( V^{(N)}_{0,n_+}(z) \) substantially differ from the 1D Coulomb potential. In the first approximation with respect to the small parameter \( a_m/a_\parallel = \gamma_\parallel^{-1/2} \), one can use the 1D Coulomb potential instead of the true effective potential. Thus the problem is reduced to finding odd-parity solutions for the 1D H atom. Formally it corresponds to setting \( z_0 = 0 \) and \( \tilde{\nu} \) to integers in Sect. VI A 1. The review of the theory of the 1D H atom is given in Ref. 39. The odd-parity solutions are well-behaved, because the singularity of the potential term in the Schrödinger equation (189) is finite for such wave functions. The Whittaker functions (190) with integer \( \tilde{\nu} \) are expressed through the generalized Laguerre polynomials, \( W_{\tilde{\nu} \frac{1}{2}}(z) = (-1)^{\tilde{\nu}} x^{-\tilde{\nu}/2} L_{\tilde{\nu}}(x) / \tilde{\nu} \), and the normalized wave functions become

\[
g_{\nu_\parallel}(z) \approx g_{\nu_\parallel}^{(0)}(z) = \sqrt{\frac{2}{a_\parallel \tilde{\nu}\tilde{\nu}!}} z \exp \left( -\frac{|z|}{\tilde{\nu} a_\parallel} \right) L_{\tilde{\nu}} \left( \frac{2|z|}{\tilde{\nu} a_\parallel} \right) ,
\]

(212)

where \( \tilde{\nu} = (\nu_\parallel + 1)/2 = 1, 2, 3, \ldots \) and \( \nu_\parallel \) is an odd longitudinal quantum number. This solution does not depend on the state of motion of the ion. Such dependence can be revealed by the perturbation theory. To the first order,

\[
E_n^{||} = -\frac{\hbar^2}{2m_\parallel a_\parallel^2} \tilde{\nu}^2 + \int_{-\infty}^{\infty} \delta V^{(N)}(z) \left[ g_{\nu_\parallel}^{(0)}(z) \right]^2 dz ,
\]

(213)

where

\[
\delta V^{(N)}(z) = V^{(N)}_{0,n_+}(z) + \frac{Z e^2}{|z|} ,
\]

(214)

is the perturbation potential. Since the integrand is non-negative, the energy levels are shifted upwards.

5. Continuum states

For positive longitudinal energies, the exterior solution is obtained by analogy with Sect. VI A 1 with a replacement \( \tilde{\nu} \to \tilde{\nu} \), where \( \tilde{\nu} \) is defined by Eq. (192) with positive \( E_n^{||} \). According to this definition,

\[
\tilde{\nu} = (a_\parallel k_\parallel)^{-1} ,
\]

(215)

where \( k_\parallel \) is the absolute value of the outgoing wavenumber given by Eq. (182). Instead of Eq. (190) we have two linearly independent solutions with asymptotes

\[
W_{\pm i\tilde{\nu}} \left( \pm \frac{2i z}{\tilde{\nu} a_\parallel} \right) \sim e^{\mp \tilde{\nu} z/2} \exp \left[ \pm i \left( k_\parallel z + \ln \left( 2k_\parallel z / k a_\parallel \right) \right) \right] ,
\]

(216)

at \( z \to \infty \). Then the longitudinal part \( g_\parallel(z) \) of a real wave function of definite \( z \)-parity, \( \psi_\parallel(r_+, r_-, z) = \pm e^{i\theta}(r_+, r_-), z \), normalized according to Eq. (137), is approximated at \( z > z_0 \) by

\[
g_\parallel(z) = \frac{e^{-\tilde{\nu} z/2}}{2 \sqrt{z}} \left[ W_{-i\tilde{\nu}} \left( \frac{2i z}{\tilde{\nu} a_\parallel} \right) e^{i\theta} + W_{-i\tilde{\nu}} \left( \frac{2i z}{\tilde{\nu} a_\parallel} \right) e^{-i\theta} \right] ,
\]

(217)

where the phase factor \( e^{\pm i\theta} \) has to be determined from the matching conditions at \( z = z_0 \). In Eq. (217), the prefactor is obtained assuming that the normalization integral over the interval \([-z_{\text{max}}, z_{\text{max}}]\) is negligibly small compared with the total normalization integral over \([-z_{\text{max}}, z_{\text{max}}]\).

B. Overlap integrals between even states

In the exterior region \( z > z_0 \), assuming that at least one of the longitudinal wave functions \( g_{\parallel}(z) \) or \( g_{\parallel'}(z) \) belongs to discrete spectrum (tends to zero at \( z \to \infty \)), the use of the Schrödinger equation and integration by parts leads to the identity

\[
\int_{z_0}^{\infty} g_{\parallel}(z) g_{\parallel'}(z) dz = \frac{\hbar}{2m_\parallel} g_{\parallel}(z) g_{\parallel'}(z) \frac{\eta - \eta'}{E_{\parallel} - E_{\parallel'}} \bigg|_{z = z_0} ,
\]

(218)
where η and η' are the corresponding logarithmic derivatives (188). In the limit \( E_κ → E_κ' \), we have

\[
\int_{z_0}^{∞} g_κ^2(z) = \frac{ħ}{2m_κ} \frac{∂^2 η}{∂ E_κ^2} \bigg|_{z=z_0}. \tag{219}
\]

The latter equation is used for normalization of the overlap integral (218). At \( a_m → 0 \), we have \( z_0 → 0 \), hence the integral over the interior region |z| < \( z_0 \) can be neglected. Then we have the normalized overlap integral

\[
\mathcal{L}(κ'|κ) ≈ \int_{z_0}^{∞} g_κ(z) g_κ'(z) \, dz \left[ \int_{z_0}^{∞} g_κ^2(z) \, dz \right]^{1/2} \left[ \int_{z_0}^{∞} g_κ^2(z) \, dz \right]^{1/2}. \tag{220}
\]

Using Eq. (218) for the numerator and Eq. (219) for the denominator on the right-hand side, we obtain

\[
|\mathcal{L}(κ'|κ)| = \left| \frac{η - η'}{E_κ^∥ - E_κ'} \right| \frac{∂η}{∂ E_κ} \frac{∂η'}{∂ E_κ'} \left[ z=z_0 \right]. \tag{221}
\]

Here, \( \mathcal{L} \) is defined by Eq. (218), where the subscripts are suppressed because only the terms with \( n_± = n_0± \) and \( n'_± = n'_0± \) survive in the adiabatic approximation.

Equations (192) and (197) give

\[
\frac{∂η}{∂ E_κ} = \frac{2m_κ a_κ^2 ν^3}{ħ^2} \frac{∂η}{∂ ν} = \frac{2m_κ a_κ^2 ν^3}{ħ^2} \left( \frac{π^2}{sin^2 νπ} + \frac{dΘ(ν)}{dν} \right), \tag{222}
\]

where function \( Θ \) is defined by Eq. (187). From Eq. (222), using Eqs. (202), (203) and the identity \( 1/sin^2 x = 1 + cot^2 x \), we obtain

\[
\frac{∂η}{∂ E_κ} = \frac{2m_κ a_κ^2 ν^3}{ħ^2} G_{N',n+1',\nu'}, \tag{223}
\]

where

\[
G_{N',n+1',\nu'} ≡ \left[ \left( \frac{ή}{2} \ln \frac{γ_κ}{2} - \frac{3}{2} \right) + \left( \frac{1}{2} J_{N,n+1} + Θ(ν') \right) \right]^2 + π^2 + \frac{dΘ(ν')}{dν'}. \tag{224}
\]

Although η and η' depend on \( z_0 \), their difference does not. From Eq. (202) we obtain the approximation

\[
η - η' ≈ \frac{J_{N,n+1} - J_{N,n+1}}{a_κ}. \tag{225}
\]

In summary, \( |\mathcal{L}(κ'|κ)| \) is given by Eqs. (221), (222), (223), and (224) as function of \( ν' \). In its turn, \( ν' \) is determined by Eq. (205).

1. The case of tightly bound states

For the tightly bound states \( (ν'_∥ = ν'_∥ = 0) \), we have \( 0 < ν < 1 \) and \( 0 < ν' < 1 \). In this particular case Eqs. (197) and (198) yield

\[
\frac{∂η}{∂ E_κ} = \frac{m_κ a_κ}{ħ^2} \left[ 2ν^2 + O(ν^3) \right]. \tag{226}
\]

Substitution of Eqs. (225) and (226) into Eq. (221) with the use of Eq. (192) gives

\[
\mathcal{L}^2(κ'|κ) ≈ \frac{4(J_{N,n+1} - J_{N,n+1})^2}{\left( \frac{1}{(ν')^2} - \frac{1}{ν^2} \right)^2 \left( ν^2 + 2ν' \right) \left( 2ν' \right)^2}. \tag{227}
\]

Using Eq. (209) for \( ν \) and \( ν' \), we substitute

\[
\frac{1}{ν^2} - \frac{1}{(ν')^2} ≈ 2 \left( J_{N,n+1} - J_{N,n+1} \right) ln \frac{γ_κ}{2}, \tag{228}
\]

and thus obtain

\[
\mathcal{L}^2(κ'|κ) ≈ \left( 1 + \frac{2}{ln(γ_κ/2)} \right)^{-2} \sim 1 - \frac{4}{ln γ_κ}. \tag{230}
\]

We see that the overlap integral does not depend on quantum numbers in this lowest-order approximation, valid at \( γ_κ → ∞ \). The asymptotic fractional accuracy of this approximation can be estimated from comparison of Eq. (206) with Eq. (209) as \( \sim [ln(ln γ_κ)] / ln γ_κ \).

2. Overlaps of tightly bound states with other even states

For the overlap integral between a tightly bound state \( (ν'_∥ = 0, 0 < ν < 1) \) and an even loosely-bound state \( (ν'_∥ = 2, 4, \ldots, ν'_∥ > 1) \), we keep using Eq. (220) for the first state \( |κ⟩ \) = \( |N, 0, n_−, n_+, 0⟩ \) and substitute Eq. (224) for the second state \( |κ'⟩ \) = \( |n_+, N', ν'_∥⟩ \). Recalling Eq. (202), we finally obtain

\[
\mathcal{L}^2(κ'|κ) = \frac{2}{(ν')^2} \frac{(J_{N,n+1} - J_{N,n+1})^2}{G_{N',n+1',ν'} \sqrt{ε_κ - ε'_κ}}, \tag{231}
\]

where \( G_{N',n+1',ν'} \) and \( J_{N,n+1} \) are defined in Eqs. (203) and (224), respectively.

3. The bound-free case

Equations (218) and (219) give the relation

\[
\left( \int_{z_0}^{∞} g_κ(z) g_κ'(z) \, dz \right)^2 \left( \int_{z_0}^{∞} g_κ^2(z) \, dz \right)^2 = \frac{ħ^2}{2m_κ} \frac{∂η}{∂ E_κ} \left( E_κ^∥ - E_κ' \right) \bigg|_{z=z_0}. \tag{232}
\]

In the case where the initial state \( κ \) belongs to the discrete spectrum but the final state \( κ' \) belongs to the continuum, taking into account that \( z_0 → 0 \) at \( γ_κ → ∞ \), we
can use the leading term of Eq. (217) at small \( \zeta \). It is
given by Eq. (196) with \( \psi \) replaced by \( i\tilde{\nu}' \). Using the
expression for the gamma function of imaginary argument
(cf. 22, 6.1.29)
\[
\Gamma(i\tilde{\nu}') = \sqrt{\frac{\pi}{\tilde{\nu}' \sinh \tilde{\nu}' \pi}} e^{-i\phi_{\tilde{\nu}'}}
\]  
(233)
where
\[
\phi_{\tilde{\nu}'} = \frac{\pi}{2} \text{sign} \tilde{\nu}' + \frac{1}{2i} \ln \Gamma(1 - i\tilde{\nu}') - \ln \Gamma(1 + i\tilde{\nu}')
\]  
(234)
we obtain
\[
g_{n_{\tilde{\nu}'}(0)} \approx g_{n_{\tilde{\nu}'}(0)} = \frac{e^{-\tilde{\nu}'\pi}}{z_{\text{max}}} \sinh \tilde{\nu}' \pi \frac{\zeta_{\tilde{\nu}'} = 1 - e^{-2\pi\tilde{\nu}'}}{2\pi\tilde{\nu}' z_{\text{max}}},
\]
where
\[
S_{n_{\tilde{\nu}'} = \sin^2(\phi_{\tilde{\nu}} - \theta)
\]  
(236)
and \( \theta \) is the undetermined phase factor in Eq. (217).

To find the factor \( S_{\tilde{\nu}'} \), we use the matching condition \( \eta'_{\text{ext}} = \eta'_{\text{int}} \). The derivative of the wave function \( \psi \) can be written as
\[
\frac{d g_{n_{\tilde{\nu}'}(0)}}{dz} = \frac{e^{-\tilde{\nu}'/2}}{\sqrt{z_{\text{max}}} \pi} \text{Re} \left[ e^{i\theta} \frac{d}{dz} W_{i\tilde{\nu}'} \left( -\frac{2iz}{\tilde{\nu}' a_{*}} \right) \right].
\]  
(237)
At \( z \to 0 \),
\[
\frac{d}{dz} W_{i\tilde{\nu}'} \left( -\frac{2iz}{\tilde{\nu}' a_{*}} \right) = e^{-i\tilde{\nu}'/2} \sqrt{\tilde{\nu}' \sinh \tilde{\nu}' \pi} \left[ \cosh \tilde{\nu}' \pi + \frac{i}{\pi} \sinh \tilde{\nu}' \pi \left( \ln \frac{2z}{a_{*}} - \Re \Theta(i\tilde{\nu}') + 2\gamma_{E} \right) \right],
\]  
(238)
where function \( \Theta \) is given by Eq. (193). Substitution of the last expression into Eq. (237) gives
\[
\frac{d g_{n_{\tilde{\nu}'}(0)}}{dz} = -4 \frac{e^{-\tilde{\nu}'/2}}{a_{*}} \sqrt{2z_{\text{max}}} \left[ \left( \cos \tilde{\nu}' \pi \Im \Theta(i\tilde{\nu}') \right) \cos(\pi \tilde{\nu}' - \theta)
+ \sinh \tilde{\nu}' \pi \left( \ln \frac{2z}{a_{*}} - \Re \Theta(i\tilde{\nu}') + 2\gamma_{E} \right) \sin(\pi \tilde{\nu}' - \theta) \right].
\]  
(239)
Here,
\[
\Im \Theta(i\tilde{\nu}') = \Im \left( \ln i\tilde{\nu}' - \frac{1}{2i\tilde{\nu}'} - \psi(i\tilde{\nu}') \right)
= \frac{\pi}{2} \left( 1 - \coth \pi \tilde{\nu}' \right),
\]  
(240)
where in the last equality we have used the relation \( \psi(i\tilde{\nu}') = 1/(2\tilde{\nu}') + (\pi/2) \coth \pi \tilde{\nu}' \) and have chosen the value of \( \Im \ln i\tilde{\nu}' = \pi/2 \). Dividing Eq. (239) by Eq. (235) and using Eq. (240), we thus obtain the logarithmic derivative \( \eta'_{\text{ext}} \) at small \( z = \zeta_{0} \):
\[
\eta'_{\text{ext}} = \frac{2}{a_{*}} \left[ \ln \frac{2z_{0}}{a_{*}} + \frac{\pi}{2} \text{sign} \tilde{\nu}' \frac{1 - e^{-2\pi\tilde{\nu}'}}{\cos(\phi_{\tilde{\nu}' - \theta)}
+ 2\gamma_{E} - \Re \Theta(i\tilde{\nu}') \right],
\]  
(241)
From Eq. (198) we obtain
\[
\Re \Theta(i\tilde{\nu}') = \ln \tilde{\nu}' - \Re \psi(1 + i\tilde{\nu}').
\]  
(242)
An efficient way of calculating \( \Re \Theta(i\tilde{\nu}') \) is presented in Appendix D.

By matching of \( \eta'_{\text{ext}} \), which is given by Eq. (211), to \( \eta'_{\text{int}} \), which is given by Eq. (212), we obtain
\[
\text{sign} \tilde{\nu}' \cot(\phi_{\tilde{\nu}' - \theta}) = \frac{1 - e^{-2\pi\tilde{\nu}'}}{2\pi} \left[ \ln \frac{\gamma_{s}}{2} - 3\gamma_{E}
- J_{N_{s}'n_{s}'} + 2\Re \Theta(i\tilde{\nu}'). \right]
\]  
(243)
Now the factor \( S_{\tilde{\nu}'} \) (236) is provided in the explicit form by the identity \( 1/\sin^2(\phi_{\tilde{\nu}' - \theta}) = 1 + \cot^2(\phi_{\tilde{\nu}' - \theta}) 
\]  
\[
S_{\tilde{\nu}'} = \left[ \left( 1 + \frac{(1 - e^{-2\pi\tilde{\nu}'})}{2\pi} \left[ \ln \frac{\gamma_{s}}{2}
- 3\gamma_{E} + J_{N_{s}'n_{s}'} + 2\Re \Theta(i\tilde{\nu}') \right] \right)^{-1} \right].
\]  
(244)
If the initial state is tightly bound (\( \nu_{0} = 0 \)), then we can use Eq. (220) for the factor \( \partial \eta/\partial E_{k} \) in Eq. (232). In the lowest approximation with respect to \( \tilde{\nu} \ll 1 \), we retain only the first (linear in \( \tilde{\nu} \)) term in this equation:
\[
\partial \eta/\partial E_{k} \approx \frac{m_{a}\tilde{\nu}}{2\pi} \hbar^2.
\]  
(232)
For the functions \( g_{k} \) and \( g_{k} \) of equal parity, the denominator on the left-hand side of Eq. (232) is approximately \( \int_{z_{0}}^{z_{\text{max}}} g_{k}^{2}(z) \, dz \approx \frac{1}{2} \int_{-\infty}^{z_{\text{max}}} g_{k}^{2}(z) \, dz \approx \frac{1}{2} \) because of the normalization condition (137), while the numerator is
\[
\left( \int_{z_{0}}^{z_{\text{max}}} g_{k}(z) g_{k}(z) \, dz \right)^{2} \approx \left[ \frac{1}{2} L^{2}(k'|\kappa) \right]^{2} = \frac{1}{4} \left( \frac{1}{k'} \right)^{2} \]  
(245)
for the same normalization. Thus Eq. (232) can be rewritten as
\[
L^{2}(k'|\kappa) = \frac{\hbar^{4} g_{k}^{2}(z_{0})}{m_{a}^{2} k^{2}} \left( \frac{(\eta' - \eta)|_{\tilde{\nu}' = 0}}{E_{k}^{\|} - E_{k}^{\perp}} \right)^{2}
\]  
(246)
Using also Eq. (235) for \( g_{s}^{2}(z_{0}) \) and Eq. (225) for \( (\eta' - \eta) \) in Eq. (232), we obtain
\[
L^{2}(k'|\kappa) = \frac{\hbar^{4}}{m_{a}^{2}} \left( \frac{1 - e^{-2\pi\tilde{\nu}'}}{2\pi z_{\text{max}} \tilde{\nu}' \hbar} \left( \frac{J_{N_{s}'n_{s}'} - J_{N_{s}'n_{s}'}}{E_{k}^{\|} - E_{k}^{\perp}} \right)^{2} S_{k'}
\]  
(247)
We recall that \( \tilde{\nu} \) and \( \tilde{\nu}' \) are defined by Eq. (192) and Eq. (215) respectively, the numbers \( J_{N_{s}'n_{s}'} \) and \( J_{N_{s}'n_{s}'} \) are given by Eq. (203), \( a_{*} \) is defined by Eq. (191), and \( S_{k'} \) is provided by Eqs. (244) and (242).

C. Transverse geometric size

In the adiabatic approximation, Eq. (145) reduces to
\[
\langle \kappa | r_{+}^{2} | \kappa \rangle = 2 a_{m}^{2} \sum_{k=0}^{N} (k + 1 + n_{-}) \left( C_{k}^{N_{s}'n_{s}'} \right)^{2}.
\]  
(248)
This equation shows that the transverse size of the ion increases with increasing \( N \). In classical physics, this increase corresponds to the action of the electric field, induced in the reference frame comoving with the ion. The forces on the nucleus and the electron, caused by this field, have opposite directions and therefore tend to stretch the ion along the radius. Since on the average \( N \) is proportional to the square of transverse momentum of the transverse motion of the ion as a whole, this stretching tends to enhance with an increase of \( N \).

One can show (see Appendix E) that

\[
\sum_{k=0}^{N} k \left( \frac{C_k^{(N,n+1)}}{C_k^{(N,n+1)}} \right)^2 = \frac{Z - 1}{Z} (N - n_+) + \frac{n_+}{Z}. \tag{249}
\]

In the most important case of the helium ion, the right-hand side of Eq. (249) reduces to \( N/2 \).

Using Eq. (249) and the normalization condition (113), we can simplify Eq. (247). Recalling that the true bound states in the ultrastrong fields exist only for \( n_+ = 0 \), for these states we obtain

\[
\langle \kappa | \mathbf{r}^2 \perp | \kappa \rangle = 2 \alpha_m^2 \left( 1 + \frac{Z - 1}{Z} (N - n_+) + \frac{n_+}{Z} \right) \tag{250}
\]

In particular, for the helium ion \( (Z = 2) \) \( \langle \kappa | \mathbf{r}^2 \perp | \kappa \rangle = (2 + N)a_m^2 \) is independent of \( n_+ \).

### D. Radiative transitions for circular polarization

In the adiabatic approximation, expressions (184) and (185) for the circular components of the dipole matrix element for the radiative transitions from state \( |i\rangle = |\kappa\rangle \) to state \( |f\rangle = |\kappa'\rangle \) with \( n_+ = n'_+ = 0 \) reduce to

\[
D_{fi,-\alpha} = \sqrt{Z n_+^{\max} \mathcal{L}(\kappa'\kappa)} \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}, \tag{251}
\]

where \( \alpha = \pm 1, n_+^{\max} = \text{max}(n_+, n'_+) \), and the overlap integral \( \mathcal{L}(\kappa'\kappa) \) is given by Eq. (221).

For the transitions between tightly-bound states (\( \nu'_\parallel = \nu_\parallel = 0 \)), Eqs. (177), (251), and (250) give the following approximate expression for the oscillator strength to the leading order in \( 1/\ln \gamma_\star \):

\[
f_{fi,\alpha} = \frac{\hbar \omega}{R \alpha_B^2} Z n_+^{\max} \left( 1 - \frac{4}{\ln \gamma_\star} \right) \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}, \tag{252}
\]

and Eq. (178) yields

\[
\sigma_{1f}^{\text{bf}}(\omega) = 4 \pi^2 \alpha_f \alpha_m^2 Z n_+^{\max} \left( 1 - \frac{4}{\ln \gamma_\star} \right) \omega \Delta_{fi}(\omega - \omega_{fi}) \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}, \tag{253}
\]

where \( \alpha_f \) is the fine structure constant. Figure 4 presents some examples of the transition energies and oscillator strengths for radiative transitions between different tightly-bound states in the dipole adiabatic approximation, according to Eq. (252).

For the bound-free transitions, substitution of Eq. (251) into Eq. (172) gives

\[
\sigma_{1f}^{\text{bf}}(\omega) = \frac{4 \pi Z n_+^{\max} m_e \omega_e \alpha_f^2}{\hbar^2 c k_f} \Delta_{fi}(\omega - \omega_{fi}) \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}, \tag{254}
\]

where \( k_f \equiv k_{\kappa'} \) is the longitudinal wavenumber defined by Eq. (155). Using Eq. (247), we obtain

\[
\sigma_{1f}^{\text{bf}}(\omega) = 2 Z n_+^{\max} \frac{\hbar^2 \omega_a^2}{m_e c k_f a_m^2 \nu} \left( 1 - \exp \left( \frac{-2 \pi \alpha_f k_f}{\hbar} \right) \right) S_c \left( \frac{J_{N'\kappa'} - J_{N\kappa}}{E_f - E_i} \right)^2 \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}. \tag{255}
\]

Taking into account definitions of \( \gamma_\star \) (207), \( \nu' \) (213), and \( \alpha_f = e^2/\hbar c \), we can write Eq. (255) in the form

\[
\sigma_{1f}^{\text{bf}}(\omega) = 2 \alpha_f Z n_+^{\max} \frac{\hbar^2 \omega_a^2}{m_e \gamma_\star \nu} \left[ 1 - \exp \left( -\frac{2 \pi \alpha_f k_f}{\hbar} \right) \right] S_c \left( \frac{J_{N'\kappa'} - J_{N\kappa}}{E_f - E_i} \right)^2 \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}. \tag{256}
\]

Using notations (192) and (193), we can also rewrite it as

\[
\sigma_{1f}^{\text{bf}}(\omega) = 4 \alpha_f n_+^{\max} \alpha_m^2 \frac{\hbar \omega}{R \gamma_\star} \left[ 1 - \exp \left( -\frac{2 \pi}{\sqrt{\epsilon_f}} \right) \right] S_f \sqrt{\epsilon_i} \left( \frac{J_{N'\kappa'} - J_{N\kappa}}{E_f - E_i} \right)^2 \delta_{n_+^\prime,n_++\alpha} \delta_{N',N+\alpha}. \tag{257}
\]

Here we have used the relation \( k_f a_m = \sqrt{\epsilon_f} \), which follows from Eqs. (155), (191), (192), and (193). Note that both
FIG. 4: Resonance transition energies $E_f - E_i$ (upper panels) and oscillator strengths $f_{fi,α}$ (lower panels) for transitions between tightly-bound states $|i⟩ = |N, n−, n+, ν⟩$ ($n− = 0, ν = 0$) and $|f⟩ = |N', n''−, n''+, ν'⟩$ ($n''− = 0, ν' = 0$) with $N' = N + 1$ and $n''_+ = n_+ + 1$ in the adiabatic approximation according to Eq. (252), as functions of magnetic field strength $B$, for $N = 0$ (solid lines), 1 (long-dash-dot lines), 2 (short-dash-dot lines), 3 (long dashes), and 4 (short dashes). Left panels: $n_+ = 0$; right panels: $n_+ = N$. The lines are terminated at the points where the final state crosses the continuum and becomes autoionizing ($E_f = 0$).

$\epsilon_i$ and $\epsilon_f$ are positive by definition. The energy conservation law requires that $E_{fi} = E_i + \hbar \omega$. Therefore, according to Eqs. (117) and (44), for the allowed dipole transitions ($n'_+ = n_+ + α$) we have $\hbar \omega / R_y = \epsilon_f + \epsilon_i + 2αγ.s$.

Examples of the photoionization cross sections, given by Eq. (257) for the circular polarizations $α = ±1$, are presented in Figs. 5-8. Figures 5, 6, and 7 correspond to the field strengths $B = 10^{12}$, $10^{13}$, and $10^{14}$ G, respectively. For $α = +1$, cross sections for the four smallest values of $n_+$ and the four smallest possible values of $N$ at each $n_+$ are shown. For $α = −1$, there are no lines with $n_+ = 0$, because absorption of photons with this polarization by such states is forbidden in the adiabatic dipole approximation. In Fig. 8 for $B = 5 \times 10^{14}$ G, only $n_+ = 0$ and $n_+ = 1$ are considered, because the states with $n_+ > 1$ have positive energies $E_i$ at such strong field. Although they can be treated as bound states in the adiabatic approximation, they actually belong to the continuum and can autoionize due to admixtures of the Landau orbitals with smaller $n_+$.

Each cross section in Figs. 5-8 decreases with increasing photon energy $\hbar \omega$ above the photoionization threshold $\hbar \omega_{thr} = −E_i = |E_i| + α\hbar \omega_{ci}$, where the longitudinal

$\hbar \omega_{thr} = −E_i = |E_i| + α\hbar \omega_{ci}$, where the longitudinal

FIG. 5: Photoionization cross sections $σ_{fi,α}(\omega)$ for different initial tightly-bound states $|i⟩ = |N, n−, n+, ν⟩$ ($n− = 0, ν = 0$) at $B = 10^{12}$ G in the adiabatic approximation according to Eq. (257) for the right ($α = +1$, the left panel) and left ($α = −1$, right panel) circular polarizations as functions of the photon energy $\hbar \omega$ in units of Thomson cross section $σ_T = (8\pi / 3)(e^2 / m_e c^2)^2$. The results are displayed for initial states with quantum numbers $n_+ = 0$ (solid lines), 1 (dot-dashed lines), 2 (dashed lines), and 3 (dotted lines) and $N = n_+, n_+ + 1, n_+ + 2, n_+ + 3$ (lines of the same type from top to bottom for each $n_+$).

FIG. 6: The same as in Fig. 5 but for $B = 10^{13}$ G.
energies $E_i^\parallel$ are calculated according to the approximation (204). The cross sections for the circular polarization become smaller with increasing magnetic field strength $B$, in agreement with the decrease of the geometric transverse cross section of the ion, which is proportional to $a_m^2 \propto B^{-1}$ (cf. Sect. VI C). The photoionization cross sections also become smaller with increasing $N$ at fixed $n_+$ and $\omega$.

VII. CONCLUSIONS

We performed a systematic derivation of practical equations for computing the basic characteristics of a one-electron ion in different quantum states in a strong magnetic field: its binding energies, geometric sizes, oscillator strengths of bound-bound transitions, and photoionization cross sections. These quantities are necessary ingredients for construction of models of atmospheres of neutron stars with strong magnetic fields under the conditions where one-electron ions can contribute substantially into the atmospheric opacities. We did not assume that the atomic nucleus is infinitely massive or fixed in space, but considered the full quantum-mechanical two-body problem. This is especially important in sufficiently warm atmospheres with sufficiently strong magnetic fields, where the thermal motion of the ions cannot be decoupled from their internal quantum-mechanical structure and the Rabi-Landau quantization of both the electron and the nucleus must be taken into account. The obtained results generally confirm, somewhat correct and extend the previously published quantum-mechanical studies of an one-electron ion, which moves in a quantizing magnetic field.

In addition, we performed an approximate analytic treatment of the problem 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 analytic expressions can be useful in the case of superstrong magnetic fields, typical for magnetars.

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Appendices

A. Supplementary relations for $C_{k}^{(N,n_{+})}$

Let us consider the operator

$$\mathcal{B} \equiv \frac{1}{\sqrt{Z}} \left( \sqrt{Z - 1} \hat{b} + \hat{a} \right), \quad (A1)$$

where $\hat{b}$ and $\hat{a}$ are defined by Eqs. (70) and (72). It follows from Eqs. (71) and (72) that

$$[\mathcal{B}, \mathcal{B}^{\dagger}] = 1. \quad (A2)$$

Besides, from Eqs. (70) and (72) we see that

$$\mathcal{B}^{\dagger} \mathcal{B} = \frac{a_{m}^{2}}{2Z\hbar^{2}}(\Pi_{\perp} - k_{\perp})^{2} - \frac{1}{2}. \quad (A3)$$

Therefore, the eigenvalues of the operator $\mathcal{B}^{\dagger} \mathcal{B}$ on the transverse basis states $|\Psi_{N,n,L}^{\perp}\rangle$ equal $n_{+}$:

$$\mathcal{B}^{\dagger} \mathcal{B} |\Psi_{N,n,L}^{\perp}\rangle = n_{+} |\Psi_{N,n,L}^{\perp}\rangle. \quad (A4)$$

Taking the commutation relation (A2) into account, we conclude that $\mathcal{B}^{\dagger}$ raises $n_{+}$ by one, while $\mathcal{B}$ decreases $n_{+}$ by one (it can be proved explicitly using Eqs. (81)). On the other hand, using the explicit form of the basis wave functions (102) and the definition of $\mathcal{B}$, we obtain

$$\mathcal{B} |\tilde{N}', L, n_{-}, n_{+}\rangle = \sum_{k=0}^{N} \mathcal{F}_{N-k-1,N}^{(Z-1)}(r_{+}, -) \mathcal{F}_{n_{-}, k}^{(-1)}(r_{-} - r_{+}) \left( \sqrt{\frac{Z - 1}{Z}} \sqrt{N - k} C_{k}^{(N,n_{+})} + \sqrt{\frac{k + 1}{Z}} C_{k+1}^{(N,n_{+})} \right). \quad (A5)$$

Therefore

$$\sqrt{n_{+}} C_{k}^{(N-1,n_{+}-1)} = \sqrt{\frac{Z - 1}{Z}} \sqrt{N - k} C_{k}^{(N,n_{+})} + \sqrt{\frac{k + 1}{Z}} C_{k+1}^{(N,n_{+})} \quad (A6)$$

In the same way, by considering $\mathcal{B}^{\dagger} |\tilde{N}', L, n_{-}, n_{+}\rangle$, we find that

$$\sqrt{n_{+} + 1} C_{k}^{(N+1,n_{+}+1)} = \sqrt{\frac{Z - 1}{Z}} \sqrt{N + 1 - k} C_{k}^{(N,n_{+})} + \sqrt{\frac{k}{Z}} C_{k-1}^{(N,n_{+})}. \quad (A7)$$

Furthermore, let us consider operator

$$\tilde{\mathcal{B}} \equiv \frac{1}{\sqrt{Z}} \left( \sqrt{Z - 1} \hat{a} - \hat{b} \right). \quad (A8)$$

It is also easy to see that $[\tilde{\mathcal{B}}, \tilde{\mathcal{B}}^{\dagger}] = 1$ and

$$\tilde{\mathcal{B}}^{\dagger} \tilde{\mathcal{B}} = \hat{b}^{\dagger} \hat{b} + \hat{a}^{\dagger} \hat{a} - \frac{a_{m}^{2} Z}{2\hbar^{2}} (\Pi_{\perp} - k_{\perp})^{2} + \frac{1}{2}. \quad (A9)$$

Therefore, the eigenvalues of the operator $\tilde{\mathcal{B}}^{\dagger} \tilde{\mathcal{B}}$ on the transverse basis states equal $N$. Taking into account the commutation relations, we obtain that $\tilde{\mathcal{B}}^{\dagger}$ and $\tilde{\mathcal{B}}$ are the creation and annihilation operators with respect to the quantum number $N + \tilde{n} - n_{+} = N - n_{+}$. By analogy with the case of operator $\mathcal{B}$ above, we obtain the following recurrent relations:

$$\sqrt{N - n_{+}} C_{k}^{(N-1,n_{+})} = \sqrt{\frac{N - k}{Z}} C_{k}^{(N,n_{+})} - \sqrt{\frac{Z - 1}{Z}} \sqrt{\frac{k + 1}{Z}} C_{k+1}^{(N,n_{+})}, \quad (A10)$$

$$\sqrt{N - n_{+} + 1} C_{k}^{(N+1,n_{+})} = \sqrt{\frac{N + 1 - k}{Z}} C_{k}^{(N,n_{+})} - \sqrt{\frac{Z - 1}{Z}} \sqrt{\frac{k}{Z}} C_{k-1}^{(N,n_{+})}. \quad (A11)$$
In the particular case $n_+ = 0$, relation (A3) gives $\sqrt{N-k} \sqrt{Z-1} C^{(N,0)}_k = -\sqrt{k+1} C^{(N,0)}_{k+1}$, which after $k$ iterations yields
\[ C^{(N,0)}_k = (-1)^k (Z - 1)^{k/2} \sqrt{\frac{N!}{k!(N-k)!}}. \] (A12)

Here, $C^{(N,0)}_0$ can be found using Eq. (A11) at $k = n_+ = 0$, $C^{(N+1,0)}_0 = C^{(N,0)}_0 / \sqrt{Z}$, which yields $C^{(N,0)}_0 = C^{(0,0)}_0 / Z^{N/2} = 1/Z^{N/2}$. The result can be written in the form
\[ C^{(N,0)}_k = (-1)^k (Z - 1)^{k/2} \sqrt{\frac{N!}{k!(N-k)!}} \equiv (-1)^k (Z - 1)^{k/2} \sqrt{\binom{N}{k}}, \] (A13)

Now, using Eq. (A7), we can find $C^{(N,n_+)}_k$ with different $n_+$.

### B. Proof of Equation (202)

The substitution of Eq. (201) into Eq. (201) gives
\[ \eta_{int}(z) \approx -\frac{2}{a_e} \int_0^{z/a_m} \int_0^{\infty} \frac{1}{k!} \left( C^{(N,n_+)}_k \right)^2 \frac{\rho^{k+\rho}}{\sqrt{\rho+\zeta}} \, d\rho. \] (B1)

Interchanging the summation and integration orders, we obtain
\[ \eta_{int}(z) \approx -\frac{2}{a_e} \int_0^{z/a_m} \frac{1}{k!} \left( C^{(N,n_+)}_k \right)^2 \int_0^{\infty} \rho^{k+\rho} \left[ \ln \left( \zeta + \sqrt{\rho+\zeta} \right) - \frac{1}{2} \ln \rho \right] d\rho \]
\[ = -\frac{2}{a_e} \sum_{k=0}^{N} \left( C^{(N,n_+)}_k \right)^2 \left[ \ln \zeta + \frac{1}{k!} \int_0^{\infty} \rho^{k+\rho} \ln \left( 1 + \sqrt{1 + \rho^2} \right) d\rho - \frac{1}{2k!} \int_0^{\infty} \rho^{k+\rho} \ln \rho d\rho \right]. \] (B2)

The first integral in the square brackets can be evaluated at $\zeta \gg 1$ as $k! \ln 2 + O(\zeta^{-2})$. The last integral equals \( [34], \) 4.352
\[ \int_0^{\infty} \rho^{k+\rho} \ln \rho d\rho = -k! \psi(k) = k! (H_k - \gamma_E), \] (B3)

where $\psi(k)$ is the digamma function \( [195] \) and $H_k = \sum_{n=1}^{k} n^{-1}$ is the $k$th harmonic number. Taking into account the normalization of $C^{(N,n_+)}_k$ \( [Eq. (39)] \) and setting $z = z_0$, we obtain Eq. (202).

### C. Estimate of $J_{N,0}$ at large $N$

Let us consider Eq. (203) at $n_+ = 0$ and $N \gg 1$:
\[ J_{N,0} = \frac{1}{Z^N} \sum_{k=1}^{N} H_k (Z - 1)^k \binom{N}{k}, \] (C1)

where we have used Eq. (A13) for $\left( C^{(N,0)}_k \right)^2$. According to the Stirling’s approximation for factorials,
\[ \binom{N}{k} \sim \left( \frac{1}{(k/N)\ln N - (1 - k/N)} + o(1) \right)^N. \] (C2)

This function is strongly peaked at $k \approx N/2$. Therefore, we can take out $H_k$ at $k \approx N/2$ from under the sum sign and obtain (for $N \gg 1$)
\[ J_{N,0} \approx \frac{H_{N/2}}{Z^N} \sum_{k=1}^{N} \binom{N}{k} (Z - 1)^k \approx \frac{H_{N/2}}{Z^N} \sum_{k=0}^{N} \binom{N}{k} (Z - 1)^k = H_{N/2} \frac{(1 + (Z - 1))^N}{Z^N} = H_{[N/2]}. \] (C3)
Now from the double inequality \[ \frac{1}{2(k+1)} < H_k - \ln k - \gamma_E < \frac{1}{2k} \] (C4)
we have \( H_{[N/2]} = \ln N - \ln 2 + \gamma_E + O(1/N) \) and
\[ J_{N_0} \sim \ln N + O(1). \] (C5)

D. Calculation of \( \text{Re} \Theta(i\tilde{\nu}) \)

The function \( \text{Re} \Theta(i\tilde{\nu}) \), which is given by Eq. (242), can be represented as (e.g., [22], 6.3.17)
\[
\text{Re} \Theta(i\tilde{\nu}) = \ln \tilde{\nu} + \gamma_E - \sum_{k=1}^{\infty} \frac{1}{k(k^2 + (\tilde{\nu})^2)} = \ln \tilde{\nu} + \gamma_E - \sum_{k=1}^{\infty} \frac{1}{k(1 + \epsilon k^2)},
\] (D1)
where \( \epsilon \) is the dimensionless longitudinal energy defined by Eq. (192). At large \( \epsilon \) (small \( \tilde{\nu} \)) the series on the right-hand side converges well, but with decreasing \( \epsilon \) the convergence becomes progressively slower, which can be easily understood from the fact that the series diverges logarithmically at \( \epsilon \to 0 \). At this limit, one can use the formula (e.g., [22], 6.3.19)
\[
\text{Re} \psi(1 + i\tilde{\nu}) = \ln \tilde{\nu} + \sum_{n=1}^{\infty} \frac{(-1)^{n-1}B_{2n}}{2n\tilde{\nu}^{2n}}.
\] (D2)
where \( B_{2n} \) are the Bernoulli numbers. However, due to the asymptotic nature of the latter formula, its accuracy rapidly worsens with increasing \( \epsilon \) at any fixed number of terms.

In this appendix we propose a method to calculate \( \text{Re} \Theta(i\tilde{\nu}) \) with keeping the number of terms of the sum in Eq. (D1) reasonably small at intermediate \( \epsilon \). Let us consider the integral
\[
\int_{-K}^{\infty} f_\epsilon(x) \, dx = \frac{1}{2} \ln \left( 1 + \frac{1}{\epsilon K^2} \right), \quad \text{where} \quad f_\epsilon(x) = \frac{1}{x(1 + \epsilon x^2)}.
\] (D3)
According to the first mean value theorem for integrals,
\[
\exists \xi_k : k < \xi_k < k + 1, \quad \int_{k}^{k+1} f_\epsilon(x) \, dx = \frac{f_\epsilon(k + 1) - f_\epsilon(k)}{2} - \frac{1}{12} f_\epsilon''(\xi_k).
\] (D4)
Assuming that \( K \in \mathbb{N} \), we can write
\[
\int_{-K}^{\infty} f_\epsilon(x) \, dx = \sum_{k=K}^{\infty} \int_{k}^{k+1} f_\epsilon(x) \, dx = \frac{f_\epsilon(K)}{2} + \sum_{k=K+1}^{\infty} f_\epsilon(k) - R_K, \quad \text{where} \quad R_K = \frac{1}{12} \sum_{k=K}^{\infty} f_\epsilon''(\xi_k).
\] (D5)
Using explicit \( f_\epsilon(x) \) in Eq. (D3), one can show that
\[
\frac{2}{\xi^2} f_\epsilon(\xi) < f_\epsilon''(\xi) < \frac{12}{\xi^2} f_\epsilon(\xi)
\] (D6)
for any \( \xi > 0 \) and \( \epsilon > 0 \). Therefore,
\[
0 < R_K < \sum_{k=K}^{\infty} \frac{1}{k^3(1 + \epsilon k^2)} < \sum_{k=K}^{\infty} \frac{1}{k^3(1 + \epsilon K^2)} < \sum_{k=K}^{\infty} \frac{1}{k^3(1 + \epsilon K^2)} = \frac{1}{2 K^2 (1 + \epsilon K^2)}.
\] (D7)
Equations (D3) and (D5) allow us to rewrite the sum on the right-hand side of Eq. (D1) as
\[
\sum_{k=1}^{\infty} \frac{1}{k(1 + \epsilon k^2)} = \sum_{k=1}^{K-1} \frac{1}{k(1 + \epsilon k^2)} + \frac{1}{2K(1 + \epsilon K^2)} + \frac{1}{2} \ln \left( 1 + \frac{1}{\epsilon K^2} \right) + R_K.
\] (D8)
Recalling that \( \dot{\nu} = 1/\sqrt{\epsilon} \) and using Eqs. (D18) and (D7), we transform Eq. (D1) into

\[
\text{Re } \Theta(i\dot{\nu}) = \gamma_E - \sum_{k=0}^{K} \frac{1}{k + c \dot{\nu}^2} + \frac{1}{2K(1 + c \dot{\nu}^2)} - \frac{1}{2} \ln \left( \epsilon + \frac{1}{K^2} \right) - \frac{a}{K^2 (1 + c \dot{\nu}^2)}, \tag{D9}
\]

where \( 0 < a < 1/2 \). This transformation allows us to greatly reduce the number \( K \) of terms in the sum, that are needed to attain a required accuracy. For example, to reproduce four digits of \( \text{Re } \Theta(i\dot{\nu}) = -0.09465 \) at \( \dot{\nu} = 1 \), we must retain more than 300 terms in the original formula (D1), while \( K = 15 \) suffices in Eq. (D9) with \( a = 0 \) and only \( K = 7 \) with \( a = 0.25 \).

In practice, we calculate \( \text{Re } \Theta(i\dot{\nu}) \) using Eq. (D9) with \( K = 3 + [11\dot{\nu}] \) and \( a = 0.25 \) at \( \dot{\nu} < 3 \) \( (\epsilon > 1/9) \). At \( \dot{\nu} \geq 3 \), we substitute Eq. (D2) retaining eight terms into Eq. (242), which gives

\[
\text{Re } \Theta(i\dot{\nu}) \approx -\frac{\epsilon}{12} - \frac{\epsilon^2}{120} - \frac{\epsilon^3}{252} - \frac{\epsilon^4}{240} - \frac{\epsilon^5}{132} - \frac{691 \epsilon^6}{32760} - \frac{\epsilon^7}{12} - \frac{3617 \epsilon^8}{8160}, \tag{D10}
\]

This recipe ensures that both absolute and fractional errors of calculated \( \text{Re } \Theta(i\dot{\nu}) \) are less than \( 10^{-6} \) for any \( \dot{\nu} \).

### E. Proof of Equation (249)

Let us rewrite equations (A6) and (A10), respectively, as

\[
\sqrt{k + 1} C_{k+1}^{(N,n_+)} = \sqrt{Z} n_+ C_k^{(N-1,n_+-1)} - \sqrt{(Z-1)(N-k)} C_k^{(N,n_+)}, \tag{E1}
\]

\[
(Z-1)\sqrt{k + 1} C_{k+1}^{(N,n_+)} = \sqrt{(Z-1)(N-k)} C_k^{(N,n_+)} - \sqrt{Z(N-1)(N-n_+)} C_k^{(N-1,n_+)}. \tag{E2}
\]

Taking the sum of the left and the right parts of these equations, we exclude the term \( \sqrt{(Z-1)(N-k)} C_k^{(N,n_+)} \) and, having divided both parts by \( Z \), obtain

\[
\sqrt{k + 1} C_{k+1}^{(N,n_+)} = \frac{n_+}{Z} C_k^{(N-1,n_+-1)} - \frac{Z-1}{Z} \sqrt{N-n_+} C_k^{(N-1,n_+)}. \tag{E3}
\]

Dropping the term with \( k = 0 \) (which equals zero) from the sum in the left-hand side of Eq. (249) and shifting the summation index \( k \) to \( k + 1 \), we can write

\[
\sum_{k=0}^{N} k \left( C_k^{(N,n_+)} \right)^2 = \sum_{k=0}^{N-1} \left( C_{k+1}^{(N,n_+)} \right)^2. \tag{E4}
\]

The substitution of Eq. (E3) gives

\[
\sum_{k=0}^{N} k \left( C_k^{(N,n_+)} \right)^2 = \sum_{k=0}^{N-1} \left( \frac{n_+}{Z} C_k^{(N-1,n_+-1)} - \frac{Z-1}{Z} \sqrt{N-n_+} C_k^{(N-1,n_+)} \right)^2 = \frac{n_+}{Z} \sum_{k=0}^{N-1} \left( C_k^{(N-1,n_+-1)} \right)^2 - \frac{2}{Z} \sqrt{(Z-1)(N-n_+)} \sum_{k=0}^{N-1} C_k^{(N-1,n_+-1)} C_k^{(N-1,n_+)}
\]

\[
+ \frac{Z-1}{Z} (N-n_+) \sum_{k=0}^{N-1} \left( C_k^{(N-1,n_+)} \right)^2. \tag{E5}
\]

According to the orthonormality relation (99), the first and third sums on the right-hand side equal one, and the second sum equals zero. Thus we are left with Eq. (249).
