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ENERGY LEVELS AND ELECTROMAGNETIC TRANSITIONS OF ATOMS IN SUPERSTRONG MAGNETIC FIELDS

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Résumé. - Lorsque les champs magnétiques appliqués à l'atome deviennent si intenses que la force de Lorentz devient comparable ou plus grande que la force de Coulomb, pour des champs \( B > 4.7 \times 10^5 \, T \cdot Z^2 \) (Z la charge du noyau), la structure atomique doit être réanalysée. Ces conditions sont celles des étoiles à neutrons. Nous présentons les résultats obtenus au cours de cette tentative, pour les systèmes à un électron (niveaux d'énergie, transitions électromagnétiques), pour les systèmes à deux électrons et l'ion \( \text{H}_2^+ \).

Abstract. - The paper reviews the results obtained so far in the endeavour to recalculate the whole of atomic physics for magnetic field strengths so strong that the Lorentz forces are comparable with or larger than the Coulomb forces, i.e. \( B > 4.7 \times 10^5 \, T \cdot Z^2 \) (Z = nuclear charge). Investigations of this kind are stimulated by the existence of such huge fields in the vicinity of neutron stars. Detailed results are presented for one-electron systems (including energy levels, electromagnetic bound-bound, bound-free, and free-free transitions), for two-electron systems, and for the \( \text{H}_2^+ \) ion.

1. Introduction. - The interpretation of the spectra of white dwarfs and accreting neutron stars confirms the existence of the huge magnetic fields associated with these compact cosmic objects. Magnetic fields of the order of \( 10^2 - 10^5 \, T \) have been observed in white dwarfs (cf. Angel et al.[1]), and of the order of \( 10^7 - 10^9 \, T \) in neutron stars (cf. Trümper[2]). On account of the prevailing physical conditions the atomic spectra of these objects should be dominated by the lines of the hydrogen-like and helium-like ions. Therefore, the accurate knowledge of the atomic properties of these ions in strong magnetic fields constitutes an essential ingredient for the detailed calculation of the ionisation equilibria, radiative processes, etc. in the atmospheres of white dwarfs and the accretion columns of X-ray pulsars. In recent years numerous investigations have been undertaken to determine the energy levels and electromagnetic transitions of hydrogen-like ions (cf.[3-11]), while for ions with more than one electron only limited results are available for energy levels, and electromagnetic transitions have not been discussed to date. The purpose of this paper is to summarize the results that have been achieved so far in the endeavour to recalculate the whole of atomic physics for magnetic fields so strong that the atomic structure is dominated by the Lorentz forces rather than by the Coulomb forces. We shall use hydrogen-like systems as a paradigm for demonstrating in detail the influence on all atomic properties and shall then consider helium-like systems. Furthermore the changes of molecular structure caused by strong magnetic fields will be discussed for the \( \text{H}_2^+ \) ion.
2. Energy levels for hydrogenic ions in arbitrary magnetic fields

a. The general two-body problem in a homogeneous magnetic field

For a system of charged particles the separation of the motion of the centre of mass by no means constitutes a problem as trivial as in the field-free case. Classically speaking every charged particle gyrates (neglecting the mutual interaction) about the magnetic field, which implies that the centre of mass does not move uniformly. This picture has led several authors to the incorrect conclusion that in the presence of a magnetic field there exists no conserved quantity for the translational motion.\[12, 13\]

For neutral systems however, it immediately follows from the translational invariance of the problem that the generalized momentum operator $P_0$, defined as the generator of an infinitesimal translation, is conserved. Taking into account that the translation must be accompanied by a gauge transformation of the vector potential $A$, one obtains $P_0$ for a neutral two-body system (charges $e_+ = e, e_- = -e$, masses $m_+, m_-)$:

$$P_0 = \frac{\hbar}{i} \frac{\partial}{\partial R} - \frac{3e}{2} B \times r.$$  \hfill (1)

where $R = (m_- r + m_+ r)/(m_- + m_+)$, $r = (r - r_0)$, and the vector potential has been chosen in the form $A(r) = 1/2 (B \times r)$. The operator $P_0$ commutes with the Hamiltonian $H$, and simultaneous eigenfunctions $\phi$ of $H$ and $P_0$ (with eigenvalues $E$ and $\hbar K$) read

$$\psi(R, r) = \exp \left[ i \frac{\hbar}{\hbar} (hK + \frac{3e}{2} B \times r) \cdot R \right] \phi(r).$$ \hfill (2)

which leads to the eigenvalue equation for the wave function $\phi(r)$:

$$H_{\text{red}} \phi(r) = \frac{\hbar^2 K^2}{2M} + (e/M)(hK \times B) \cdot r + \frac{e^2}{4\pi \epsilon_0 r} + V_\text{c}(r) \phi(r) = E \phi(r).$$ \hfill (3)

where $M = m_+ + m_-$, $\mu = (m_+ - m_+ + m_-)/M$, $p = -i\hbar \partial / \partial r$, and $V_\text{c}(r) = -e^2/(4\pi \epsilon_0 r)$ is the Coulomb interaction.

The eigenfunctions and the eigenvalues of (3) depend on $K, B, M$, and $\nu$, i.e., $\phi = \phi(K, B, M, \nu, r)$ and $E = E(K, B, M, \nu)$. A closer inspection of the structure of the Schrödinger equation (3) yields the scaling laws

$$\phi(\lambda K, B, M, \mu; r) = \lambda^{3/2} \phi(K, B/\lambda^2, M/\lambda, \mu/\lambda; \lambda r),$$ \hfill (4a)

$$E(\lambda K, B, M, \mu) = \lambda E(K, B/\lambda^2, M/\lambda, \mu/\lambda).$$ \hfill (4b)

Thus, in order to exploit the scaling freedom in the quantum number $K$, the solutions of (3) have to be known, for some given value of $K = 0$, as continuous functions of the magnetic field strength and of the masses involved. Since for strong magnetic fields these solutions can be obtained numerically only, the practical treatment of the two-body problem in the general case $K \neq 0$ constitutes a laborious task. In the following, we shall concentrate on the case $K = 0$, which represents, also in magnetic fields, the physically reasonable starting point for investigating the internal properties of two-body systems. Here the Hamiltonian in (3) becomes axially symmetric, and $\phi$ can always be chosen as an eigenfunction of $L_z = (r \times p)_z$ with eigenvalue $\hbar \mu$. Then the $M$-dependence of the energy is simply contained in a diagonal term, and the scaling laws can be formulated most conveniently in terms of the solutions of the problem for $M \rightarrow \infty$ (without loss of generality we take $m_+ \rightarrow \infty$ and abbreviate $m_+/m_- = \lambda$ )

$$\phi_\mu(m_-, m_+, B; r) = \lambda^{3/2} \phi_\mu(m_-, m_+ \rightarrow \infty, B/\lambda^2; \lambda r),$$ \hfill (5a)

$$E_\mu(m_-, m_+, B) = \lambda E_\mu(m_-, m_+ \rightarrow \infty, B/\lambda^2) - \hbar m_e B/m_+,$$ \hfill (5b)

(cf. Pavloy-Verevkin and Zhilinskii [14]). It is seen that, for a given $m_-$ and $K=0$, once the problem has been solved in the limit $m_+ \rightarrow \infty$ for every value of $B$, the
solutions of the two-body problem with mass $m_-$ and arbitrary finite values of $m_+$ are also known. From (5) the scaling law for the dipole strengths,

$$ d_{\tau',\tau}(m_-, m_+; B) = \lambda^{-2} d_{\tau',\tau}(m_-, m_+ \to \infty, B/\lambda^2), \quad \lambda = m_+/(m_+ + m_-). $$

From (5b) and (6) the scaling behavior of oscillator strengths, transition probabilities, etc., is immediately calculated. Important applications of the mass scaling laws are the hydrogen atom with finite proton mass, and positronium (cf. Wunner et al. [15]). It should be noted that, contrary to widely held opinion, the effect of the finite proton mass is not always of the anticipated order of magnitude $m_e/m_{\text{proton}}$. The last term in (5b) causes a shift between states with different $m$ by $\Delta m \cdot \text{heB/m}_{\text{proton}} \approx 29.6 \text{ eV} \cdot 4.7 \cdot 10^8 \text{T}^2$, which, in high fields, becomes comparable with the Coulomb binding energies, and thus is by no means negligible (cf. Wunner et al. [16]).

In contrast to the field-free case, the well-known Z-scaling is possible, in the presence of a magnetic field, only in the limit $m_+ \to \infty$. For the sake of completeness we list the scaling laws for the wave functions and energies:

$$ \phi_m(Z, B; r) = Z^{3/2} \phi_m(Z = 1, B/Z^2; Zr), $$

$$ E_m(Z, B) = Z^2 E_m(Z = 1, B/Z^2) $$

(cf. Surmelian and O'Connell [17]). From this we can derive the scaling laws for the dipole strengths

$$ d_{\tau',\tau}(Z, B) = Z^{-2} d_{\tau',\tau}(Z = 1, B/Z^2), $$

and analogously from (7b) and (8) those for the oscillator strengths, etc.

The practical application of the scaling for the energies and dipole strengths requires the knowledge of the continuous $B$-dependence of these quantities for $m_+ \to \infty$. A rigorous analytical solution to this problem is not possible, and a reasonable way is to solve the Schrödinger equation numerically accurate for a sufficiently dense sequence of discrete $B$ values.

### b. Solution of the Schrödinger equation for infinite proton mass

In solving the Schrödinger equation, quite generally two asymptotic ranges of the magnetic field strength have to be distinguished, namely the low-field region $B < B_Z = 2a^2 m_e c^2/(\epsilon \hbar) \approx 4.7 \cdot 10^8 \text{T} \cdot Z^2$ and the high-field region $B > B_Z$, where either the Coulomb forces or the Lorentz forces are dominant.

Our procedure for determining as accurately as possible hydrogenic wave functions in magnetic fields of arbitrary strength starts from expanding the wave functions in terms of spherical harmonics for low fields

$$ \phi_m = \sum f_{l1}(r) Y_{lm}(\theta), $$

while for high magnetic fields, where the spherical symmetry of the Coulomb potential is destroyed by the magnetic field to an ever increasing extent, the expansion in terms of Landau states $\phi_m \text{Land}_{nm}(r, \theta)$ (n: Landau quantum number, m: magnetic quantum number, see, e.g., Canuto and Ventura [18]) is more appropriate

$$ \phi_m = \sum_n g_n(Z) \phi_m \text{Land}_{nm}(r, \theta). $$
Inserting (9), or (10), into the Hamiltonian of the problem, and projecting on the different spherical harmonics, or Landau states, yields a system of integro-differential-equations for the expansion functions \( f_1(r) \), or \( g_n(z) \), which is coupled via the matrix elements of the diamagnetic term in the Hamiltonian,

\[
V_{11}^{(m)}(r) = \langle Y_{1m}(\alpha) | e^2 B^2/(8m_i) r^2 | Y_{1m}(\alpha) \rangle,
\]

or those of the Coulomb potential,

\[
V_{nn}^{(m)}(z) = \langle \phi_{nm}^{\text{Land}}(r_\alpha) | Ze^2/(4\pi\varepsilon_0 r) | \phi_{nm}^{\text{Land}}(r_\alpha) \rangle,
\]

respectively. Both systems of equations possess the mathematical structure of the Hartree-Fock equations encountered in field-free atomic physics. We therefore took the well-known Froese-Fischer code (Froese-Fischer [19]), which has proved so successful in field-free Hartree-Fock calculations, and adapted it to the requirements of the two different ranges of the magnetic field strength (Pröschel [20], Rosner [21]). By virtue of its apt choice of the integration mesh and its refined integration methods, the code is not only numerically very stable, but also very fast, and allows an inclusion of more than 10 components in (9) and (10) without any substantial expenditure of computer time or memory. The convergence of the method can be seen by successively increasing the maximum number of components included in (9) or (10). A detailed description of our numerical procedure is found in refs. [20,21].

![Figure 1.- Convergence of the results for the energy values in dependence on the maximum number \( n_k \) of configurations included in (9) and (10). The curves refer to the state with asymptotic quantum numbers \( 1s0/000 \) (a: \( \beta = 7 \), b: \( \beta = 20 \)). It is recognized that in general the spherical computation (curves marked by "s") converges more rapidly than does the cylindrical one (curves marked by "c"). For increasing \( \beta \), however, the cylindrical curves flatten, and more configurations are needed in the spherical calculation to reach saturation. The behaviour shown can be used to extrapolate the energy values to \( n_k = \infty \).

Results and discussion

As a representative example for the calculations performed by us, in Table 1 we list the energy values (in units of the Rydberg energy \( E_H = \alpha^2 m_e c^2 / 2 \approx 13.6 \text{ eV} \)) of the nine lowest \( m=0 \) states of the H atom for various magnetic field strengths in the range \( 10^{-4} \leq \beta < 10^3 \) (\( \beta = B_i / B \)). The states are labelled by both their field-free quantum numbers and their asymptotic (\( \beta \rightarrow \infty \)) quantum numbers \( n_m, \nu \) (\( \nu \) is the number of nodes of the dominant longitudinal wave function in (10) for \( \beta \rightarrow \infty \), which at the same time expresses the correspondence between the different asymptotic quantum numbers. For small fields, a subscript of the type \( N_1/N_2 \) indicates that the energy value was computed including up to \( N_2 \) components in (9), and that the significant di-
Table 1. Energies of the nine lowest m=0 states (left: positive z-parity, right: negative z-parity) of the H atom in units of the Rydberg energy for magnetic fields of arbitrary strength.

A subscript N, N indicates that the energy value was computed using up to N, configurations in (9), and that the digits given were already obtained for N, configurations. Energies Values with a single subscript N were computed including a maximum number of N configurations in (9) or (10), and the numbers following the slash mark the values to which the last digits converge if the extrapolation method of Fig. 1 is employed.

<table>
<thead>
<tr>
<th>β</th>
<th>1σ/000</th>
<th>2σ/000</th>
<th>3σ/000</th>
<th>4σ/000</th>
<th>5σ/000</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0001000</td>
<td>0.1</td>
<td>0.000010101</td>
<td>0.000010101</td>
<td>0.000010101</td>
</tr>
<tr>
<td>0.2</td>
<td>0.0002000</td>
<td>0.2</td>
<td>0.000020202</td>
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<td>0.000020202</td>
</tr>
<tr>
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<tr>
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<tr>
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<td>0.0009000</td>
<td>0.9</td>
<td>0.000090909</td>
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<tr>
<td>1.0</td>
<td>0.0010000</td>
<td>1.0</td>
<td>0.001010101</td>
<td>0.001010101</td>
<td>0.001010101</td>
</tr>
</tbody>
</table>
gits given were already obtained for $N_\ell$ components. For intermediate and strong fields, the single subscript indicates the maximum number of configurations used in the computations in (9) or (10), and the number following the slash gives the values towards which the last digits tend if use is made of the extrapolation method discussed in Fig. 1. The solid lines below certain energy values mark the boundaries from whereon the Landau expansion produces better results than the expansion in terms of spherical harmonics. The mesh of $p$-points in Table 1 is chosen in such a way that in a quadratic interpolation for intermediate $p$-values one to two significant digits at most are lost.

Comparing with the best values for the energies of these states known to date (Prad- daude [22], Cabib et al. [23] for $\beta < 2.5$, Simola and Virtamo [4] for $\beta > 2.5$), it is found that our results either reproduce their values, or even lie slightly lower on account of their higher number of significant digits. It is evident from Table 1 that the number of significant digits obtainable in the present calculations is largest in the low-field regime ($\beta < 1$); this is of course due to the fact that here the diamagnetic term in the Hamiltonian represents only a small perturbation to the field-free spherical problem. In particular, it can be verified from Table 1 that, as pointed out by Ruder et al. [24], the simple formulae of a standard perturbation calculation,

$$E_{n_p l m}/E_H = -1/n_p^2 - 2\beta + 2m\beta + \beta^2 \langle (x^2+y^2)/a_B^2 \rangle_{n_p l m},$$

(13)

where $n_p$ designates the principal quantum number, $a_B$ is the Bohr radius and

$$\langle (x^2+y^2)/a_B^2 \rangle_{n_p l m} = 2/3 < r^2/a_B^2 >_{n_p l m} \{ 1 + \frac{3m^2 - 1(1+1)}{(2l+3)(2l-1)} \}$$

(14)

with

$$< r^2/a_B^2 >_{n_p l m} = 1/2 \ n_p^2 [ 5n_p^2 + 1 - 3(1+1) ],$$

(15)

are capable of producing the correct energy values with a remarkable accuracy up to magnetic fields $\beta \sim 10^{-9}$ for the states under consideration. In the regime of intermediate field strengths, $0.1 \leq \beta \leq 10$, where the dominance of the Coulomb potential is gradually superseded by that of the magnetic field, the number of necessary angular momentum components rapidly increases. It is, however, only for $\beta > 10$ that the Landau expansions yield more accurate results using fewer configurations than would be required in the corresponding angular momentum expansion.

For illustrational purposes, in Fig. 2 the energies of several low-lying states with $m = 0, -1, -2$ are plotted as continuous functions of the magnetic field strength. Fig. 2 exhibits the well known fact that for every value of $m$ there exists one (asymptotically node-less) state which is strongly lowered in energy ("tightly bound states"), while the energies of all other states ("hydrogen-like states") are less than one Rydberg, and in the limit $\beta \to \infty$ converge to the field-free eigenvalue spectrum of the H atom (Loudon [25]). In fact, writing the energy values for finite $\beta$ and fixed $m$ in the form $E_{\nu} = -E_{\nu}/(\nu + \delta_{\nu})$, where \( \nu = \nu/2 \) for even $\nu$ and $\nu^{2} = (\nu+1)/2$ for odd $\nu$, it is found that the (formal) quantum defect $\delta_{\nu}$ rapidly tends to some constant value for even and odd $\nu$, respectively, as $\nu$ goes to infinity. This fact can be used to calculate with satisfactory accuracy, for given $\beta$ and $m$, the energies of all highly excited bound states of the H atom. It may be noted, however, that the knowledge of the energy values for $\nu > 1$ is more or less of academic interest, since the widths of these levels due to the interaction with the radiation field, or with other atoms, easily become comparable with the energies themselves.

Because of the extraordinary accuracy of their energy values, the wave functions (9) and (10) are particularly well-suited for calculating matrix elements and expectation
Figure 2.- Energies of low-lying \( m=0, -1, -2 \) states of the H atom in units of the Rydberg energy as a function of the magnetic field parameter \( \beta \). The states are labelled by their asymptotic field-free and adiabatic approximation quantum numbers.

Table 2.- Mean square radius and value of the wave function at the origin of the lowest \( m=0 \) state, and mean square radius of the lowest \( m=-1 \) state of the H atom as a function of the magnetic field strength. (For \( m=-1, \phi(0)=0 \) for all values of \( \beta \).) The subscripts indicate the number of configurations and the method used in computing the values ("a": eq.(9), "b": eq.(10). For (-1) read \( 10^{-4} \), etc.; \( a_0 \) denotes the Bohr radius.

<table>
<thead>
<tr>
<th>( \beta )</th>
<th>( \langle r^2/a_0^2 \rangle )</th>
<th>( \langle \phi^2(0) \rangle \a ) ( \langle \phi^2 \rangle \b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3.000</td>
<td>1.000</td>
</tr>
<tr>
<td>0.001</td>
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<td>2.999735643a</td>
<td>1.000037526a</td>
</tr>
<tr>
<td>0.025</td>
<td>2.996769104a</td>
<td>1.000281985a</td>
</tr>
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<td>1.033619924a</td>
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<tr>
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<td>7.415964a(-1)</td>
<td>4.06789a</td>
</tr>
<tr>
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<td>3.2326a(-1)</td>
<td>1.57196a(+1)</td>
</tr>
<tr>
<td>25</td>
<td>1.95122a(-1)</td>
<td>3.81120a(+1)</td>
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<td>1000</td>
<td>4.07312a(-3)</td>
<td>2.85128a(+3)</td>
</tr>
</tbody>
</table>

Figure 3.- Magnetic-field dependence of the ground state energy of hydrogenic uranium (non-relativistic and relativistic calculation). At \( B \approx 4.5 \times 10^{11} \) T the ground state energy reaches the lower continuum, which may result in the spontaneous production of positrons.
values, which are more sensitive to approximation methods than are energies. Table 2 provides, for various magnetic fields strengths in the range $0 < \beta < 10^3$, the mean square radii of the lowest $m = 0$ and $m = -1$ states of the H atom, and, for $m = 0$, also the value of the wave function at the origin, calculated using our multi-configuration wave functions (9) and (10). The subscripts attached to the results indicate the type of expansion ("a" for (9), "b" for (10)) and the number of configurations necessary to guarantee the numerical stability of the results with respect to all the digits given. The dramatic decline of the mean square radius, and the strong increase in the value of the $m = 0$ wave function at the nucleus, which are evident from the tabulated results, are altogether clearly indicative of the total rearrangement of atomic structure which occurs as the magnetic field increases beyond some critical value of $\beta$.

Concluding this section we note that the solution of the Dirac equation for the H atom in strong magnetic fields (Lindgren and Virtamo [26]) reveals that relativistic effects are negligible even at magnetic field strengths $B = B_c r = 4.4 \times 10^8 \text{T}$, where the level distance in the Landau spectrum becomes equal to the rest mass of the electron. This may be explained by the fact that even in the relativistic treatment the spatial dependence of the spinors as regards the motion perpendicular to the magnetic field is given by the Landau functions $\phi_{nm}^{\text{Lan}}(r_z)$, and thus for the motion parallel to the field the electron ultimately feels the same effective potentials as in the non-relativistic treatment. Relativistic corrections are therefore only of the order of the ratio of the Coulomb binding energies (a few hundreds eV for the tightly bound states) and the electronic rest mass, and thus negligible. However, relativistic effects can no longer be neglected for higher nuclear charges, where, by the Z-scaling law (7b), for tightly bound states binding energies of hundreds of keV may be obtained. For hydrogenic uranium ($Z = 92$) in Fig. 3 the relativistic energy of the ground state is plotted as a function of the magnetic field strength. It is seen that for $B > 10^9 \text{T}$ relativistic corrections indeed become sizeable, and for $B \approx 4.8 \times 10^{11} \text{T}$ the ground state plunges into the filled Dirac sea, which entails the spontaneous production of positrons [27] (decay of the vacuum). Magnetic field strengths of this magnitude are expected to occur for very short times in heavy-ion collisions [28].

3. Electromagnetic transitions of hydrogenic ions in strong magnetic fields


The calculation of electromagnetic transitions is a standard chapter of quantum mechanics, the essential formula being the famous "golden rule" (see, e.g., Heitler [29]). However the resulting final expressions for field-free transitions which may be found in atomic physics literature cannot simply be applied to atoms in strong magnetic fields. This is mainly because of the completely altered structure of atomic wave functions. Thus the recalculation of the cross sections and transition probabilities of all relevant processes is requisite.

Bound-bound transitions of hydrogenic ions in strong magnetic fields have been discussed in considerable detail by Wunner and Ruder and Wunner et al. [8] within the framework of the "adiabatic approximation". This approximation amounts to including in the Landau expansion (9) solely the contribution of $n = 0$, which is justified when the Landau level distance $4\beta E_H$ is large compared with the Coulomb binding energies, i.e. for $\beta \gg 1$. In particular, the adiabatic approximation becomes exact in the limit $\beta \to \infty$. The intuitive meaning of the adiabatic approximation is that in strong magnetic fields the motion of the electron perpendicular to the magnetic field in (undisturbed) Landau orbits is much faster than that parallel to the field, whence for this motion the electron effectively feels the Coulomb potential averaged over the Landau orbit. In fact, the longitudinal parts of the adiabatic
Figure 4.- Oscillator strengths for the H atom as a function of the magnetic field strength. Top: results obtained using perturbation theory and adiabatic approximation wave functions, crosses refer to refs.[7,30,31]. Bottom: results for intermediate field strengths obtained using multi-configuration wave functions (9) and (10).
approximation wave functions are obtained by solving one-dimensional Schrödinger equations with the effective potentials \(v_{\text{eff}}(z)\) (see (12)). The comparison of the energy values calculated in adiabatic approximation with the highly accurate ones determined with the help of the multi-configuration wave functions (10) shows that for the tightly bound states the deviations are about 1% for \(\beta = 50\), and about 0.2% for \(\beta = 10^6\), while the energies of hydrogen-like states are even more accurate by a factor of 5 to 10.

In Fig. 4a we have plotted the oscillator strengths \(f_{\tau\tau}^{(q)}\) of \((\Delta m = q)\)-transitions between low-lying states \(\tau, \tau'\) of the H atom as a function of the magnetic field strength. The values for \(\beta > 1\) have been calculated using adiabatic approximation wave functions, those for \(\beta < 10^{-2}\) using ordinary Schrödinger perturbation theory wave functions. Because of the stronger sensitivity of matrix elements to approximation methods, the adiabatic approximation curves have been dashed for \(\beta < 50\), where the accuracy is expected to become worse than \(\pm 5\%\). Additionally we have included in Fig. 5a the few values for the oscillator strengths existing in the literature for \(B \geq 10^3\) T [Smith et al. [30]; Brandi, Santos, and Miranda [31]; Kara and McDowell [7]]. It is seen that in the region of small \(\beta\) the oscillator strengths of those transitions which also occur at \(\beta = 0\) differ only slightly from the field-free values, while the oscillator strengths of the other transitions increase with a simple power law in \(\beta\) according to the removal of the energy degeneracy of the respective states. In the high-field region all oscillator strengths decrease due to the shrinking spatial extension of the atomic wave functions. The decrease in \(\Delta m \neq 0\) transitions is more pronounced since here the extension perpendicular to the magnetic field is essential, and asymptotically these oscillator strengths behave as \(1/\beta\). In order to bridge the gap in Fig. 4a where neither perturbation theory nor the adiabatic approximation is applicable, we used multi-configuration wave function (9) and (10) to calculate the relevant matrix elements. The results obtained [32] for the oscillator strengths in the range \(10^3 \leq B \leq 5 \times 10^6\) T are shown in Fig. 4b. From the convergence of the results with increasing maximum number of configurations it may be concluded that at least three significant digits can be guaranteed for the values of the oscillator strengths over the whole range of \(B\) shown in Fig. 4b. Figs. 4a and 4b clearly exhibit the total rearrangement, not only of level structure, but also of emission spectra that takes place when \(\beta\) becomes of order unity.

With the help of the scaling laws (7b) and (8), the results of Fig.4 can immediately be transferred to hydrogenic ions. With regard to applications to strongly magnetized accreting neutron stars with source temperatures \(kT \sim 10^7\) keV, hydrogen-like iron (Fe XXVI) is of particular interest. A careful estimate of the relevant physical parameters has recently led Ruder et al. [33] to the prediction that photon fluxes in the Lyman-\(\alpha\) line which should be observable with spectrometers at present or in the near future can be expected from accreting neutron stars of not too high X-ray luminosity. The fundamental importance of the actual observation of magnetically strongly shifted iron lines to the physics of neutron stars as well as to atomic physics in strong fields is evident.

### b. Bound-free transitions

To arrive at the general ionisation formula of a plasma the accurate knowledge of the cross sections of the following elementary bound-free processes are a necessary input from atomic physics: 1) photoionisation and photoionisation, 2) collisional ionisation and three-body recombination. Once the cross sections are known it can be decided under which physical conditions the electronic, or photonic, ionisation-recombination mechanism contributes dominantly to establishing the ionisation equilibria. The knowledge of the ionisation equilibria, in turn, is prerequisite to quantitatively calculating atomic line spectra (both in emission and absorption) from cosmic X-ray sources. It now becomes clear how the results of calculations for photoionisation [34] and impact ionisation [35] performed for magnetic fields \(B = 10^7\) - \(10^9\) T within the adiabatic approximation using accurate numerical longitudinal wave functions for states both in the discrete and the continuous spectrum.

Fig. 5a shows the computed photoionisation cross section of the H atom for \(B = 4.7 \times 10^8\) T for photons incident perpendicular, and with polarisation parallel, to the magnetic field. The cross section exhibits - characteristic of the presence of a magnetic field - spikes at photon energies which correspond to Landau excitations.
Figure 5a.- Total photoionisation cross section of the H atom for $B=4.7\cdot10^5$ T as a function of the photon energy (or the energy distance from the ionisation threshold) for photons incident perpendicular, and polarisation parallel, to the field (lower curve: $B=0$). The spikes in the cross section correspond to the excitation of the electron into higher Landau levels.

Figure 5b.- Same as Fig. 5a for hydrogenic iron.
The comparison with the field-free result shows that in a strong magnetic field the cross section is increased by several orders of magnitude. From Fig. 5b, where the same situation is presented for Fe XXVI, it can be seen that also for larger nuclear charges jumps are present at the Landau excitations; however, for a given magnetic field strength the difference with respect to the field-free cross section is less pronounced, caused by the stronger Coulomb forces.

Fig. 6 shows the cross section for impact ionisation of the H atom as a function of the energy of the incoming electron for $\beta = 50$ and $\beta = 10^5$. The ionisation thresholds are marked by vertical dashed lines. Comparing with the field-free result ($\beta = 0$) we see that the cross section is decreased as the magnetic field increases. The calculations have not yet been extended beyond the first Landau threshold where again spikes in the cross section will occur.

As far as the time-reversed processes are concerned it must be noted that, as a consequence of the different dimensionality of the density of final states of the electron (three-dimensional for $B = 0$, one-dimensional in the strongly magnetised case), the field-free transformation laws can no longer be applied. For example, the relation between the cross section of photorecombination of an electron with Landau quantum number $n' = 0$, and kinetic energy $E' > 0$ to a bound state with $n = 0$, and energy $E < 0$, accompanied by the emission of a photon of wave vector $\mathbf{k}$ ($\hbar \mathbf{c} = E' + |E|$) and the corresponding ionisation cross section is obtained as

$$\frac{d\sigma_{\text{rec}}}{d\Omega} = \frac{(ka_L)^2}{4\pi} O_{\text{ion}}$$

(16)

where $a_L = (2\hbar/eB)^{1/2}$ denotes Larmor quantum length, and a similar law can be derived for three-body recombination. - The question as to the predominance of one of the two ionisation-recombination mechanisms depends, of course, on the particular physical situation (electron density, photon density, temperature, etc.), and will not be pursued here.

c. Free-free transitions (bremsstrahlung)

The bremsstrahlung process is the dominant mechanism for the production of the $\gamma$-quanta emitted from the accretion columns of neutron stars. The elementary bremsstrahlung cross section therefore enters as a local source term into every self-consistent radiative transfer calculation which aims at the correct description of the emitted continuous X-ray spectrum. Starting point of our own numerical calculations [36] for magnetic fields $B < 10^6 - 10^7$ T were the attempts undertaken previously by Canuto et al. [37], Virtamo and Jauho [38], and Akopyan and Tsytovich [39]. Our results were obtained for electrons moving freely parallel to the magnetic field (Born's approximation), and in Landau orbits perpendicular to the field. Furthermore it was assumed that the electrons occupy the lowest Landau level ($n = n' = 0$) both in the initial and the final state. For a magnetic field of $4.4 \times 10^6$ T Fig. 7 shows, in an exemplary way, the differential cross section per energy interval of the emitted photon for the energy $E_e$ of the electron in the initial state of 10%, or 90%, of the Landau level distance $\Delta E_{\text{L}}$, respectively. For every value of $E_e$ 4 curves are shown, corresponding to the 2 polarisations of the photon, and to the 2 possibilities of whether or not the direction of the z-momentum of the electron is reversed. It is seen that in general the backward process is suppressed with respect to the forward process; furthermore, for small electron energies polarisation of the photon in the $k$-$B$-plane is predominant, while for electron energies closer to the Landau threshold polarisation perpendicular to the $k$-$B$-plane becomes more and more favourable as the photon energy increases. Folding the cross section with a given electron distribution function leads to the photon spectrum produced by the elementary bremsstrahlung process. It must be stressed, however, that, in an optically thick plasma, the ultimately emitted spectrum may still be reprocessed by the interaction of the bremsstrahlung quanta with other electrons (Comptonisation).

4. Two-electron systems in strong magnetic fields

The starting point for treating higher atoms in strong magnetic fields is the level
Figure 6.- Total cross section for impact ionisation of the H atom in strong magnetic fields as a function of the energy of the incoming electron. For comparison, the field-free cross section is also shown. The dashed lines mark the ionisation thresholds.

Figure 7.- Energy distribution of the bremsstrahlung quanta in a magnetic field $B=4.4 \cdot 10^8$ T for two values of the energy $E$ of the electron in the initial state ($\omega_B = eB/m_e$).

On account of the one-dimensionality enforced by the magnetic field, in the process only the component of the electron momentum parallel to the field is altered (solid lines: no change of direction, dashed lines: change of direction; 1: polarisation of the photon in the $k-B$ plane, 2: polarisation perpendicular to the $k-B$ plane).

Figure 8.- Ground state energy of He as a function of the magnetic field parameter $\beta_2$. Solid curve: SCHF calculation in adiabatic approximation [40], dashed curve: spherical MCHF calculation (ls2p, $^3P_1$, + ls4f, $^3P_1$ with inclusion of the diamagnetic term [42].
scheme of the H atom, where, in a single-particle picture, the lowest states 
\(m = 0, -1, \ldots\) are consecutively occupied by the atomic electrons. Evidently the ca-
nonical approach to the problem is a Hartree–Fock (HF) calculation in which for every single-particle wave function an expansion (10) in terms of Landau orbitals is taken, and the \(z\)-dependent expansion functions are determined selfconsistently 
in the course of a MCHF procedure. A simpler situation arises if the conditions for the adiabatic approximation \((B > B_z, \text{i.e. } \beta_z = B/B_z > 1)\) are fulfilled; then the 
single-particle wave functions can reasonably be described by products of Landau 
states and longitudinal functions,

\[
\phi_i(i) = \phi_{n_i=0,m_i}^{\text{Landau}}(r_{i\perp}) \cdot g_{m_i} \phi_i(z_i),
\]

and the many-electron wave function is represented by a single Slater determinant. 

The general Hartree–Fock equations in adiabatic approximation, together with appli-
cations to the isoelectronic sequence of He (up to Fe XXV), have recently been 
treated in detail by Pröschel et al. [40], who employed an adopted version [20] of the 
successful Froese–Fischer code [19] for solving the HF equations. As one example, 
the magnetic-field dependence obtained for the ground state energy of He is shown 
in Fig. 8 (solid curve for \(\beta_z > 1\)); the energy-lowering effect of strong magnetic 
fields on ground states is evident again. Note that, in particular, the lowest state 
becomes a triplet state. Fig. 8 also contains (dashed curve) the results of MCHF 
calculations in a spherical basis which selfconsistently took into account the dia-
magnetic Hamiltonian [42]; it is found that this procedure operates remarkably well 
even up to \(\beta_z > 20\), and, for \(\beta_z > 1\), lies below the adiabatic approximation results. 

This is of course due to the fact that a single Slater determinant cannot account 
for correlations between the electrons included in MCHF wave functions. 

Obviously the next step will be to calculate energies and wave functions of excited 
states of helium-like systems in strong magnetic fields within Hartree–Fock theory, and, 
then, to evaluate the matrix elements of electromagnetic transitions between 
these states. Furthermore a quantitative investigation also of lithium-like systems 
in strong magnetic fields will become numerically feasible. In addition, the exten-
sion of the method to multi-Landau-configuration forms of the \(N\)-electron wave func-
tion can be envisaged.

5. The \(\text{H}_2^+\) ion in strong magnetic fields

As a final point, let us briefly discuss the behaviour of the simplest molecular 
structure - the \(\text{H}_2^+\) ion - in strong magnetic fields. Investigations of the \(\text{H}_2\)system 
in the high-field regime are of particular interest as they can serve as a useful 
guide to studying quantitatively linear polyatomic chains in superstrong magnetic 
fields, which are expected to play an important role for the solid state structure 
of neutron star surfaces. References to the existing literature may be found in 
Wunner et al. [43], where energy values, equilibrium internuclear separations, and 
zero-point energies of nuclear vibrations parallel to the field were calculated 
for the lowest states using the adiabatic approximation. 

It is evident that a consistent description of the \(\text{H}_2^+\) ion from first principles 
would require the solution of the quantum-mechanical three-body problem in the pre-
ance of a magnetic field. Apart from the formidable difficulties encountered al-
ready in the field-free case, this task is additionally complicated by the fact that 
for charged systems in magnetic fields the total momentum is no longer a conserved 
quantity[44]. Lacking a satisfactory solution to this problem, most of the authors 
have considered the electron moving in the Coulomb fields of two protons located at 
fixed positions \(z_A = -R/2, z_B = +R/2\) on the \(z\)-axis, taken to point along the direc-
tion of the magnetic field.

As an example Fig. 9 shows the energy curves of the lowest \(m = 0\) and \(m = -1\) state 
of the \(\text{H}_2^+\) ion for various values of the magnetic field parameter \(\beta = B/4.7 \times 10^6 \text{T}\) . 

It is seen that, as the magnetic field increases, the energy curves become stiffer 
and stiffer, the equilibrium internuclear distance is shifted to smaller values, 
and the energy at minimum is strongly lowered. In particular, as an effect of the
strong magnetic field, states that do not bind in the field-free case, such as the lowest \( m = -1 \) state, become binding for \( \beta \neq 0 \).

![Diagram showing energy as a function of internuclear separation for various magnetic field parameters.](image)

**Figure 9.** - Energy of the lowest \( m=0 \) and \( m=-1 \) state of the \( \text{H}_2^+ \) ion as a function of the internuclear separation \( R \) (in atomic units) for various values of the magnetic field parameter \( \beta \). As \( \beta \) increases, the equilibrium distance is shifted to smaller values, and the binding energy strongly increases; in particular, the anti-binding \( m=-1 \) state becomes a binding state.

It is easy to see that the configuration of the \( \text{H}_2^+ \) ion with the molecular axis parallel to the magnetic field represents an energetic minimum. A perturbation theory estimate shows, however, that the zero-point energies associated with the vibrations of the nuclei perpendicular to the magnetic field for sufficiently large \( \beta \) may become of the same order of magnitude as the Coulomb binding energies. Obviously the Born-Oppenheimer approximation breaks down in such a situation. Furthermore, the effects associated with the finite mass of the protons and the net singly positive charge of the system are estimated to be of the order of the proton cyclotron energy, and thus are expected to lead to nonnegligible corrections to the binding energy in the high-field regime. This once again illustrates the fact that the treatment of atomic and molecular systems in strong magnetic fields, motivated by the discovery of such fields in compact cosmic objects, still raises a number of unanswered, though fascinating, quantum mechanical problems - problems that should be tackled in the near future.

**References**

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