SOME PROPERTIES OF ONE ELECTRON ATOMS IN INTENSE MAGNETIC FIELDS

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M.R.C. McDowell

Mathematics Department, Royal Holloway College,(University of London),Egham Hill, Egham, Surrey TW20 OEX, U.K.

Résumé. - Les propriétés des systèmes à un électron dans un champ magnétique intense sont tout d'abord passées en revue. Un travail récent sur les états liés et sur les transitions entre états liés est ensuite discuté ainsi que le problème de l'espacement des niveaux d'énergie associés au mouvement transverse, dans le continuum. De nouveaux résultats sur la variation de cet espacement avec z sont présentés dans le cas d'un champ d'intensité 10^7G, pour m = -1. On montre que les états de nombre quantique principal n $\leq$ 5 deviennent "liés" pour z petit. Ceci est interprété en termes d'ionisation par champ. Des lois d'échelle pour la diffusion d'électrons par des cibles à un électron sont ensuite rapidement discutées.

Abstract. - The properties of one electron systems in intense magnetic fields are reviewed. Recent work on bound states and bound-bound transitions is discussed, as is the problem of the energy level spacing for the perpendicular motion in the continuum. New results are presented for the variation of this spacing with z in the case of a field of 10^7G, for m = -1. It is shown that states with Landau quantum number n $\leq$ 5 become "bound" at small z. This is interpreted in terms of field ionisation. Scaling laws for electron scattering by one electron targets are briefly discussed.

1. <u>Introduction</u>. - We consider some properties of one-electron atoms in intense magnetic fields. Relativistic effects are neglected.

We first discuss the bound states and their scaling. This leads on to a discussion of the bound-bound transition probabilities, and their scaling. The main new results concern an adiabatic approximation to the energies and wave functions of the quasi-Landau levels embedded in the continuum. Some remarks are made on photoionisation, and recent exact and approximate scaling laws for this process reviewed. The problem of electron scattering by one electron targets in a magnetic field is discussed, and it is shown that the first Born approximation is valid for all energies at sufficiently high nuclear charge.

2. <u>Bound states and energy levels</u>. - We consider a uniform static magnetic field $\underline{B}$ along the z-axis, and choose cylindrical polar coordinates $(\rho,\theta,\bar{z})$. We write

$$\underline{B} = B \hat{\underline{z}} \tag{1}$$

with

$$\gamma = \frac{B}{B_o} , \qquad B_o = 2.3505 \ 10^5 T \qquad (2)$$

and suppose that the mass of the nucleus may be taken as infinite. Finite mass effects are significant at very high fields $(\gamma \gg 1)$ and have been considered by, among others, Herold et al[1]. We take the nuclear charge as $\alpha_o e$. The Schrödinger equation is

$$H \Psi = E \Psi \qquad (3)$$

with

$$H = - \frac{1}{2} \nabla^2 - \frac{\alpha_o}{r} + \frac{1}{2} \gamma L_z + \frac{1}{8} \gamma^2 \rho^2 \qquad (4)$$

and the eigenfunctions Ψ have a conserved value m of azimuthal quantum number and parity π. We may put

$$\Psi(\underline{r}) = \rho^{-\frac{1}{2}} f(\rho, z) e^{im\theta} \qquad (5)$$

to obtain

$$\left\{ \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial z^2} - V_m(\rho, z) + E' \right\} f(\rho, z) = 0 \qquad (6)$$

with

$$E' = E - \gamma m \quad (Ry)$$

and

$$V_m(\rho, z) = \frac{(m^2 - \frac{1}{4})}{\rho^2} - \frac{2\alpha_o}{(\rho^2 + z^2)^{\frac{1}{2}}} + \frac{1}{4} \gamma^2 \rho^2 . \qquad (8)$$

The boundary conditions are

$$f(0, z) = 0, \quad f(\infty, z) \to 0$$

and in general we consider quadratically integrable solutions. The differential equation (6) is of course non-separable, and recourse must be had to approximate methods. Work up to 1975 has been reviewed by Garstang[2], and we will comment only on some recent results. For weak fields the quadratic Zeeman term $\frac{1}{4} \gamma^2 \rho^2$ may be treated as a perturbation. For very high fields $(\gamma \gg 1)$ the Coulomb term $- \frac{2\alpha_o}{r}$ may be considered as the perturbation and an expansion made in terms of Landau functions. At intermediate field strengths, $\gamma \sim 1$, variational methods are available, either in terms of specified basis functions, or in a Hartree-Fock approach. Here $\gamma = \gamma(\alpha_o = 1)$ and we will see later that it must be scaled for $\alpha_o \neq 1$. Most calculations are confined to the lowest fourteen levels, that is those which go to the nth level, $n \leq 3$. However Patil[17] has recently given analytic expressions for the high field energies of states with $n \geq 3$. At low fields we may label the energies by the quantum numbers $(n \ell m)$ as in the field free case. The results (Schiff and Snyder[3]) have recently been compared with variational calculations by Ruder et al[4]. The perturbation calculation is accurate for the ground state to better than 1% for $\gamma_1 < 0.43$ and to better than 0.7% for all these states at $\gamma_1 = 4.3 \ 10^{-3}$ when compared with the variational calculations of Kara and McDowell[5]. The $|3s_o>$ and $|3d_o>$ states

combine as

$$|3s_0'> \ = 0.402 \ |3s_0> + 0.916 \ |3d_0> \left.\begin{array}{l} \\ \\ \end{array}\right\}$$

$$|3d_0'> \ = 0.916 \ |3s_0> - 0.402 \ |3d_0> \ . \tag{9}$$

The tabulated values omit the finite mass correction term which is of order $1.5 \ 10^{-6} \ \gamma m(eV) \simeq 10^{-7} \ \gamma m$ Ry.

A mixed variation-perturbation calculation which uses only two variational parameters by Cohen and Herman[6] for $|1s_0>$, $|2s_0>$, $|2p_0>$, $|2p \pm 1>$ fails badly for $|2s_0>$ at $\gamma_1 = 0.43$.

The adiabatic approximation has been used by Simola and Vertamo[7] and by Wunner[8] and polynomial approximations to the energy levels given by Wunner and Ruder[9]. They give results for $\gamma < 2 \times 10^4$. The states are labelled by the Landau quantum numbers (n,m) and the number ν of nodes in the longitudinal wave function. For odd, but not for even, ν the energies approach the infinite-field limit by $\gamma \sim 2 \times 10^4$. Wunner and Ruder[9] use these results to compute the wave lengths of the Balmer series lines in fields appropriate to neutron stars. An alternative approach has been used by Bender et al[18] for the lowest state of each m. They expand

$$E = \frac{\gamma}{\eta^2} \sum_{s=1}^{\infty} E_s k^{-s}$$

with $k = 2 (|m| + 1)$ and η is a dimensionless parameter related to the minimum of $V_m (\rho,z)$. They obtain analytic expressions for E_{-1} through E_2.

As was first shown by Surmelian and O'Connell[10] the energies scale as

$$E_j(\alpha_0,B) = \alpha_0^2 E_j(1,B/\alpha_0^2) \tag{10}$$

and the wave functions as

$$\psi_j(\alpha_0,B,\underline{r}) = \alpha_0^{3/2} \psi_j(1,B/\alpha_0^2,\alpha_0\underline{r}) \tag{11}$$

as may readily be proved from (1) and (2). Thus non-relativistic energies are known for the lowest fourteen states for the entire iso-electronic sequence. Fig. 1 shows the variation of the lowest energy levels with field strength $(\alpha_0 = 1)$.
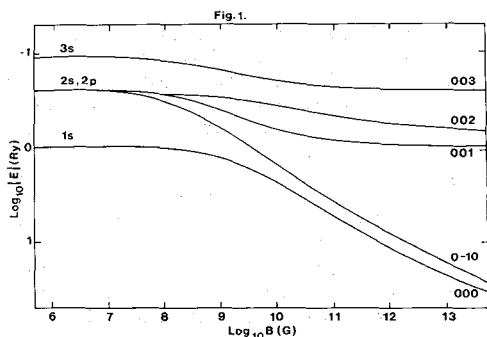

Fig. 1.

Fig. 1

The six lowest lying levels of atomic hydrogen as a function of magnetic field strength. B (Gauss) (after Ruder et al[4]).

3. <u>Dipole matrix elements and oscillator strengths</u>. - Einstein A_{ij} coefficients and oscillator strengths of transitions connecting the lowest fourteen levels have been given by a number of authors (Brandi et al[11], Smith et al[12], Kara and McDowell[5], Wunner et al[13], Wadehra[14]). The results are in general in close agreement, and those for six transitions are shown in Fig. 2, adopted from ref. (13).
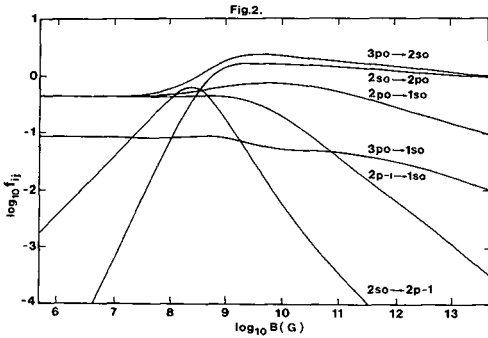

Fig. 2

Oscillator strengths for transitions among the low lying levels of atomic hydrogen as a function of field strength (after Ruder et al[4].

It is important to note that $f_{nn'}$ can vary by almost five orders of magnitude when γ changes by a factor of 100! This is, in particular, the case for the $|2s_0> \rightarrow |2p_0>$ transition. The discordant results of ref. (11) and ref. (8) for the very weak $|3d \pm 1> \rightarrow |3p \pm 1>$ transitions have been resolved by Ruder et al[4] in favour of Brandi et al[11]. Wunner et al[13] show that the dipole matrix element scales as

$$d_{n'n}(\alpha_0, B) = \alpha_0^{-2} d_{n'n}(1, B/\alpha_0^2) \qquad (12)$$

so that the oscillator strength scales as[15]

$$f_{n'n}(\alpha_0, B) = f_{n'n}(1, B/\alpha_0^2) \qquad (13)$$

as might have been expected in view of the sum rule.

These results have been used by Ruder et al[15] to discuss the spectrum of H-like iron (Fe XXVI) in neutron star accretion layers where fields of order 10^{11} to 10^{13} G may be present. This corresponds to effective fields γ in the range $0.1 \leq \gamma \leq 10$. The Ly line has a photon energy increasing from 7 keV at 10^{11} G to 21 keV at 10^{13} G and a lifetime of order 10^{-15} s.

A quite different approach is required for the Rydberg levels, and has been discussed by Clark and Taylor in a number of papers(16). Since they will be discussing their work in detail at this meeting we merely note here that they consider states near the ionisation limit, where the ionisation potential is of the same order as the cyclotron energy. They use a very large Sturmian function basis and obtain the eigenvalues for $n \geq 23$, and corresponding oscillator strengths, to a resolution of 0.1 cm^{-1} at 4.7 T. No study has yet been made of the variation of oscillator strength with field, but we would anticipate significant variation when $\Delta\gamma \sim 0 (\Delta E_{nn'})$. At $n = 23$, $\Delta E_{n,n+1} \sim 1.5$ 10^{-4} Ry and at 4.7 T, $\gamma = 4.25 \ 10^{-6}$ Ry, so one would not expect much change between n manifolds for small field changes. However, we would expect significant variation among the Balmer emission lines from a given n.

4. <u>Continuum levels</u>. - Much less is known about the continuum levels of one-electron systems in magnetic fields. The photoabsorption experiments of Garton and Tomkins[19], Garton et al[20], Castro et al[21], Gay et al[22] and Delande and Gay[23] appear to show a level spacing just above the ionisation threshold of $\Delta E_{n,n+1} \simeq 3\gamma$ Ry. The spacing expected in the absence of the Coulomb interaction is of course 2γ Ry, the Landau spacing. The explanation was first given by Edmonds[24]. He argued that near $E = 0$ the semi-classical frequency associated with motion along the z-axis was small compared with that of the cyclotron motion, and evaluated the energy in a plane perpendicular to z using a JWKB approximation,

$$\int_{\rho_1}^{\rho_2} \left[E_n + \frac{1}{(\rho^2 + z^2)^{\frac{1}{2}}} - \frac{1}{2\rho^2} (m + \frac{1}{2} \gamma \rho^2)^2 \right]^{\frac{1}{2}} d\rho = \frac{\pi}{\sqrt{2}} (n + \frac{1}{2}) \qquad (14)$$

where n is the number of nodes in the radial wave function; ρ_i the classical turning points. The Landau spacing is recovered when $z \gg \rho$, but for small z he found $(dE/dn)^{-1} \simeq 3.16\gamma$ Ry. This work was later refined by Starace[25] and Rau[26]. Very recently Gallas and O'Connell[27] have shown, following Starace and Rau, that for the motion in the $z = 0$ plane, the energy spacing can be expressed analytically in terms of complete elliptic integrals, of the first and third kinds. Applications to the experimental spacings in Rb have been reported by Economou et al[28] and to Ba and Sr by Fonck et al[29]. There is no need to make the JWKB approximation: Kara and McDowell[30] have solved (6) directly for $z = 0$. Their results for two cases are compared in Table 1. The spacings found are appreciably different from the JWKB Coulomb-Landau limit. It is well known that

<div align="center">Table 1</div>

(1) $B = 10^7$ G , $m = -1$

n	$E_n{}'$	$E_n{}'$ (JWKB)	ΔE
7	2.726	2.717	
8	5.317	5.309	2.60
9	7.796	7.789	2.48

(2) $B = 5 \times 10^8$, $m = -1$

n	$E_n{}'$	$E_n{}'$ (JWKB)	ΔE
1	0.309		2.35
2	2.661	2.643	2.21
3	4.872	4.857	2.15
4	7.020	7.006	

Exact solutions of eqn. (6) in the $z = 0$ plane compared with JWKB values. ΔE is the level separation. All quantities are in units of γ Ry.

$\Delta E_{n,n+1}^{(m,\pi)} \to 2\gamma$ Ry as n becomes large. What had not fully been appreciated before the Kara and McDowell calculations was that there are no solutions for $n < n_{min} (\gamma)$ for the motion perpendicular to the z-axis. Thus Kara and McDowell found (Table 1) that many quasi-Landau levels were missing in the $z = 0$ plane at fields below 10^9 G. These states certainly exist as $z \to \infty$: they are the field-free Landau levels. Further, n is here the number of radial nodes in the perpendicular motion, and is conserved as we vary z. We can attempt to trace these states adiabatically, and write (6) as

Table 2

m	B(G)	10^7	10^8	5×10^8	10^9
-1		6	3	1	1
0		7	3	2	2
1		6	2	1	0

Minimum value of n for the perpendicular motion in the $z = 0$ plane at different fields.

$$\left\{ \frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial z^2} - V_m (\rho, z_0) + E'_m \right\} \zeta (z) F_{z_0} (\rho) = 0 \qquad (15)$$

for fixed $z = z_0$. We assume the radial wave function $F_{z_0}(\rho)$ is a slowly varying function of z and neglect $F_z = \partial F_{z_0}(\rho) \partial z$ and $F_{zz} = \partial^2 F_{z_0}(\rho)/\partial z^2$. That is, we assume $<F_z>$ and $<F_{zz}> << k_z^2$ where $<>$ indicate averages over ρ for fixed $z = z_0$. This remains to be confirmed. Integrating outwards from the origin we can obtain a starting series by putting

$$r^{-1} \simeq \frac{1}{z_0} [1 - \tfrac{1}{2}\rho^2/z_0^2 + \cdots] . \qquad (16)$$

To find the eigenvalues for fixed Landau quantum number n, we either start at $z = 0$ with Kara and McDowell's values, or at very large z with the Landau value. Nuzzo and McDowell[31] have carried out calculations initially for $B = 10^7$ G and $m = -1$. Further work is in hand. The results to date are shown in Fig. 3. For $n = 7$ and $n = 6$ the energy of the perpendicular motion decreases smoothly from the Landau value with decreasing z to the $z = 0$ limit. However, for $n = 5$ for which no $z = 0$ eigenvalue with $E > 0$ was found, $E_5(z)$ changes sign near $z_0 = 4.0$ and goes to a $z_0 = 0$ limiting value of $\sim 2.095 \gamma$ Ry. Note that this lies almost exactly 3γ Ry below the first continuum state $(n = 6)$: here $\gamma = 0.0043$, so at $z_0 = 0$ the $n = 5$ state lies just over 100 meV below the ionisation threshold. It follows that the states with $n = 0, 1, 2, 3, 4$ lie below this at spacings of about 0.17 eV, and thus we predict the $n = 0$ state to be bound by about 1 eV at $z_0 = 0$. Within the limits of our adiabatic approximation, which remains to be tested, this appears to mean that the very high lying Rydberg states are in effect field ionised by the magnetic field. This might be directly testable at fields of 100 T (10^6 G) where the binding of the $n = 0$ level should be about 0.1 eV, provided this is much greater than $k_0 T$.
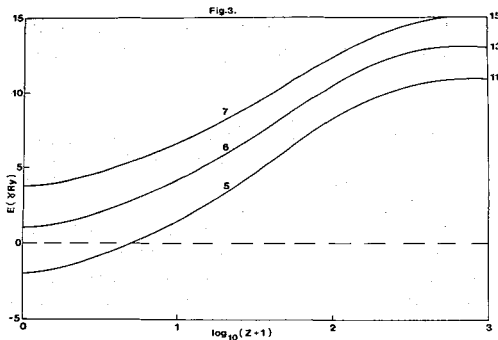

Fig. 3

The adiabatic energies of motion perpendicular to the field in the $n = 5, 6, 7$ states of $m = -1$ of the continuum at a field $\gamma = 0.0043$ (10^7 G).

5. <u>Photoionisation</u>. - The photoionisation cross section is given by[30]

$$a_\nu = 8.59 \ 10^{-19} \ h\nu \sum_{n=n_{min}}^{n_{max}} |S_{if}| \ \frac{L_z}{4\pi k_z} \ cm^2 \qquad (17)$$

where we adopt a quantisation length of L_z along the field. The density of states is

$$\rho(E_z) = \frac{L_z}{2\pi} \cdot \frac{1}{2k_z}$$

where $E_z = k_z^2$ is the energy of the ejected electron in Rydbergs, and S_{if} is the dipole matrix element. Calculations have been made by Ruder[32] and his colleagues for Fe XXVI at very high fields ($\gamma \gg 1$) using an adiabatic approximation for the continuum wave function

$$\Psi_{n,m,k_z^2}(\underline{r}) = \phi_{nm}^{(L)}(\rho,\phi) g_{nmk_z^2}(z) \qquad (18)$$

where the z-component is obtained by solving

$$\left\{\frac{d^2}{dz^2} + k^2 + <\phi_{nm}^{(L)}| \ \frac{2\alpha_0}{r} \ |\phi_{nm}^{(L)}>\right\} g_{nmk_z^2} = 0 \qquad (19)$$

with the boundary condition of no outgoing wave at $z = -\infty$ and regular and irregular solutions

$$g^\pm \underset{|z| \to \infty}{\sim} e^{\pm ikz} \ exp\left\{\pm \frac{L}{k_z} \ln k_z z\right\} . \qquad (20)$$

They use the full electromagnetic Hamiltonian and do not make the dipole approximation, but restrict themselves to photoionisation into the first Landau level. A scaling law[37] then allows them to write down the result for any one electron system

with $\qquad \sigma(\alpha_0,B,E,E',\underline{k}) = \alpha_0^{-1} \ \sigma(1,B\alpha_0^{-2},E\alpha_0^{-2},E'\alpha_0^{-2},\underline{k}\alpha_0^{-1}) \qquad (21)$

$$E + \hbar k c = E'.$$

Kara and McDowell[30] have made similar calculations at intermediate field strengths 10^7 to 10^9 G ($0.0043 \leq \gamma \leq 0.43$) for photoionisation from both the $1s_0>$ and $|2p_0>$ states, using accurate ground state wave functions. For the continuum wave functions they choose

$$\Psi_{n,m,k_z^2}(\underline{r}) = C \ \rho^{-\frac{1}{2}} f_n(\rho,o) \ e^{ik_z z} \ e^{im\phi}. \qquad (22)$$

Because of the choice of $z = z_0$ they found the main resonant behaviour at the thresholds of the bound states of perpendicular motion in the $z = 0$ plane, rather than at the Landau energies ($z \to \infty$). The discussion in section 4 above suggests that since these energies vary with z some sort of averaging procedure will be needed to obtain accurate results. Kara and McDowell found, following Blumberg et al[33] that the cross section behaved near threshold as k_z for $|\Delta m| = 1$ transitions but as k_z^{-1} for $|\Delta m| = 0$ odd parity bound states, and the reverse for even parity bound states. They used the dipole approximate scaling law[37] for which the simple scaling law[37]

$$a_\nu(\alpha_0,B) = \alpha_0^{-2} \ a_{\nu'}(1,B/\alpha_0^2) \qquad (23)$$

with

$$\nu' = \nu/\alpha_0^2 \qquad (24)$$

applies. There are no available measurements except those of Blumberg et al[33] on S^-, but both experiment and theory for H^- are in hand.

6. <u>Scattering of electrons by one electron targets</u>. - McDowell[34]
has recently reviewed the work to date on the scattering problem, and
attempted to derive scaling laws. Using the uni-dimensional density
of final states for the scattered electron the cross section for the
transition in which the incident electron makes a transition from a
continuum state $|n_i m_i k_i>$ to a final continuum state $|n_f m_f k_f>$ while
the target goes from initial bound state $|n_i^{(b)} \ell_i m_{\ell_i}>$ to
$|n_i^{(b)} \ell_i m_{\ell_i}>$ to $|n_f^{(b)} \ell_f m_{\ell_f}>$ is[35]

$$\sigma_{if}(k_i^2) = \frac{L_z^2}{k_i k_f} |<f|T|i>|^2 . \tag{25}$$

The only detailed calculations to date are by Ohsaki[36] who considers

$$e^- + H(1s) \rightarrow e^- + H(1s, 2s, 2p)$$
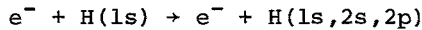
at fields of 10^8 and 10^9 Gauss and impact energies up to 90 eV.
Unfortunately he uses unperturbed wave functions, which are of
doubtful value for the ground state at such fields, and totally
unreliable for the excited states. In addition he carries out the
calculation in the First Born Approximation (FBA) which is unlikely to
be valid at such energies. His quantitative results are thus unlikely
to be correct but the main qualitative feature may be. The incident
and scattered electron are, in FBA, represented by unperturbed Landau
functions so he finds large resonant enhancements of the excitation
cross when the $k_f^2 = (\Delta E_{if} + 2j\gamma)$ Ry, $j = 1, 2, 3 \ldots$.

Consider an electron scattered by a one-electron target of nuclear
charge α_0. The bound electron sees the full nuclear charge, but the
incident electron sees only the residual Coulomb field of charge
$(\alpha_0 - 1)$. We can therefore partition the Hamiltonian as

$$H = \left[\Pi_1^2 - \frac{(\alpha_0 - 1)}{r_1}\right] + \left[\Pi_2^2 - \frac{\alpha_0}{r_1}\right] - \frac{1}{r_1} + \frac{1}{r_{12}} \tag{26}$$

where $\underline{\Pi}_i$ is the full momentum $(i = 1,2)$.

In FBA the T-matrix is, neglecting exchange,

$$T_{if}^{BI} = <\Psi(n_i m_i k_i; \underline{r}_1) \Psi(n_i^{(b)} \ell_i m_{\ell_i}; \underline{r}_2) \left| \frac{1}{r_{12}} - \frac{1}{r_1} \right|$$

$$\Psi(n_f m_f k_f; \underline{r}_1) \Psi(n_f^{(b)} m_{\ell_f} \ell_f | \underline{r}_2) > \tag{27}$$

where $\Psi(\cdots; \underline{r}_1)$ satisfies (3) with charge $(\alpha_0 - 1)$ and
$\Psi(\cdots; \underline{r}_2)$ with charge α_0. It is clear that no simple scaling law
exists. An approximate result may be obtained when $\alpha_0 \gg 1$. The FBA
matrix element scales as α_0, so for the nuclear charges $\alpha_1, \alpha_2 \gg 1$,
hence for incident energies $k_i^2 = \alpha_i^2 k^2$ and fields $B_i = \alpha_i^2 B$
$(i = 1,2)$,

$$\sigma_{if}^{BI}(\alpha_1, k_1, B_1) = \alpha_1^{-2} C_{if}$$

and

$$\sigma_{if}^{B2}(\alpha_2, k_2, B_2) = \alpha_2^{-2} C_{if}$$

so

$$\alpha_1^2 \sigma_{if}^{BI}(\alpha_1, k_1, B_1) = \alpha_2^2 \sigma_{if}^{B2}(\alpha_2, k_2, B_2) . \tag{28}$$

The second Born term $<i|V \, G_0^+|V>$ scales independent of charge, since the Green's function G_0^+ scales as α_0^{-2}; the third and higher terms go as α_0^{-1}, α_0^{-2}, ... etc. That is, provided $\alpha_0 \gg 1$, the Born series is an expansion in α_0^{-1}. Thus for sufficient large charge (28) is true for the full cross section to a good approximation, <u>at all energies</u>

$$\alpha_1^2 \, \sigma_{if}^{B1} \simeq \alpha_1^2 \, \sigma_{if}(\alpha_1, k_1, B_1) \simeq \alpha_2^2 \, \sigma_{if}(\alpha_2, k_2, B_2) \; . \qquad (29)$$

In the case of atomic hydrogen alone, where the continuum electron see the magnetic field modified by a short range field it may be a satis-factory approximation to represent this electron by a Landau function. This is not true when the residual charge $(\alpha_0 - 1)$ is non-zero: then the solutions of (3) must be used for both electrons. Detailed calculations will be very difficult, as cross sections for the atomic processes must be summed over all allowable final quasi-Landau states and averaged over all initial quasi-Landau states. Presumably for transitions in, e.g. hydrogen-like iron, which are of interest for astrophysical purposes, one could assume a Boltzmann distribution of electron energies, but it is not clear how these should be partitioned among quasi-Landau levels.

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