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HYDROGEN ATOM IN A STRONG MAGNETIC FIELD: BOUND-BOUND TRANSITIONS*

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ABSTRACT

Bound-bound transition probabilities are calculated for a hydrogen atom, in magnetic fields from 10^7 to 10^8 gauss.

Subject headings: magnetic fields — neutron stars — transition probabilities — white-dwarf stars — Zeeman effect

The discovery of pulsars and magnetic white dwarfs (Kemp 1970*a*, *b*; Kemp *et al.* 1970) has stimulated interest (Cohen, Lodenquai, and Ruderman 1970; Mueller, Rao, and Spruch 1971; Rajagopal *et al.* 1972; Smith *et al.* 1972) in the behavior of atoms in strong magnetic fields $B \approx 10^6$–10^{13} gauss. The most difficult region to investigate is where the Coulomb and magnetic field forces are of comparable strength ($B \approx 10^7$–10^{11} gauss). The energy spectrum of the hydrogen atom has now been determined (Rajagopal *et al.* 1972; Smith *et al.* 1972) in such fields by variational techniques. It was found that all the eigenstates can be labeled $\psi_m{}^{\pm}$, where m and $\pm$ are the eigenvalues of the z-component of the orbital angular momentum L, and parity, respectively. This contrasts with the low-field case of the normal Zeeman effect, where perturbation theory holds and n, L, and m are all good quantum numbers. For arbitrary fields, each state $\psi_m{}^{\pm}$ can be expanded in terms of spherical harmonics of order l, with l even for even parity and odd for odd parity.

These results (Rajagopal *et al.* 1972; Smith *et al.* 1972) are of relevance for the calculation of astrophysically interesting effects, such as opacities in magnetic white dwarfs and pulsars. As an initial step, in the execution of such a program, we present bound-bound transition probabilities.

The Hamiltonian for a hydrogen atom in a magnetic field B oriented along the z-axis is (neglecting spin)

$$H_0 = \frac{p^2}{2\mu} - \frac{e^2}{r} + \omega_L L_z + \tfrac{1}{2}\mu\omega_L{}^2 r^2 \sin^2\theta\,, \tag{1}$$

where the Larmor frequency is $\omega_L = eB/2\mu c$.

When radiation terms are included in the Hamiltonian, the interaction term which causes transitions is given by

$$H_{\rm I} = \frac{e}{\mu c}\boldsymbol{A}\cdot(\boldsymbol{p} + \mu\omega_L\hat{B}\times\boldsymbol{r})\,, \tag{2}$$

where $\boldsymbol{A}$ is the vector potential for the radiation field.

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In the electric-dipole approximation, the probability per unit time for an atom to undergo a transition from state m to m' and emit light of frequency $\omega_{m'm} = (E_m - E_{m'})/\hbar$, in the polarization direction $\hat{e}_q$ into a solid angle $d\Omega$ is

$$A_{m'm}d\Omega = \frac{e^2\hbar}{2\pi\mu^2c^3}\,\omega_{m'm}\left|\left\langle m'\left|\left(\nabla + i\frac{\mu}{\hbar}\,\omega_L\hat{B} \times r\right)\cdot\hat{e}_q{}^*\right|m\right\rangle\right|^2 d\Omega\,. \quad (3)$$

The unit directions $\hat{e}_q$ are defined by

$$\hat{e}_{\pm 1} = \mp 2^{-1/2}(\hat{e}_x \pm i\hat{e}_y)\,; \qquad \hat{e}_0 = \hat{e}_z\,,$$

where $\hat{e}_x$, $\hat{e}_y$, and $\hat{e}_z$ are unit vectors along the x, y, and z directions, respectively.

We may rewrite equation (3) in terms of the familiar dipole-length matrix element $\boldsymbol{R}_{m'm} = \langle m'|\boldsymbol{r}|m\rangle$ by using the commutation relation

$$[\boldsymbol{r}, H_0]_{m'm} = \frac{\hbar^2}{\mu}\langle m'|\nabla|m\rangle - \hbar(m' - m)\omega_L\langle m'|\boldsymbol{r}|m\rangle$$
$$= (E_m - E_{m'})\langle m'|\boldsymbol{r}|m\rangle\,. \quad (4)$$

Hence,

$$A_{m'm}d\Omega = \frac{e^2}{2\pi\hbar c^3}\,\omega_{m'm}{}^3(1 + 2f)^2|\boldsymbol{R}_{m'm}\cdot\hat{e}_q{}^*|^2 d\Omega\,, \quad (5)$$

where

$$f \equiv (m' - m)(\omega_L/\omega_{m'm})\,. \quad (6)$$

Thus we see that terms additional to that proportional to $\omega_{m'm}{}^3$ arise in the presence of an external magnetic field.

The energy spectrum for an H atom in a magnetic field is obtained from the eigenvalues of the Hamiltonian operator given in equation (1). A general form of the trial solution may be written

$$\psi_m{}^{\pm}(\boldsymbol{r}) \equiv \psi_t = \sum_{il}[a_i{}^{(t)}r^l + b_i{}^{(t)}r^{l+1}]\exp[-\beta_i{}^{(t)}r]\,Y_{lm}(\theta, \phi)\,, \quad (7)$$

where $a_i{}^{(t)}$, $b_i{}^{(t)}$, and $\beta_i{}^{(t)}$ are parameters. The sum on l in equation (7) over all even integers leads to the state with even parity (+); the sum over odd l, to the odd-parity (−) state. Here m is the eigenvalue of L_z.

The quadratic Zeeman effect mixes states such as $l = 0$ and $l = 2$, and so interference effects can appear, for example, in the Balmer series where the lower state has $l = 0$ and $l = 1$. We have automatically taken into account these mixing effects by summing over l in equation (7). Note that only m and parity are now good quantum numbers. Thus Smith *et al.* (1972) were able to obtain the exact energy eigenvalues for the 14 lowest states of the hydrogen atom.

For convenience, we display in figure 1 the energy spectrum (Smith *et al.* 1972) for B fields from 10^7 to 10^8 gauss, except that we have omitted the ground state $1s_0$, since its value is essentially constant at −13.6 eV over this range. The labeling of the curves corresponds to the usual labels for the hydrogenic energy levels in the absence of a magnetic field. Thus, for example, $3d_2$ is an even-parity state with $m = 2$, and, as $B \to 0$, it also has $n = 3$ and $l = 2$.

For spontaneous emission in the dipole approximation, we have two of the usual selection rules, viz., parity change and $\Delta m = 0$ or ± 1. We have calculated transition

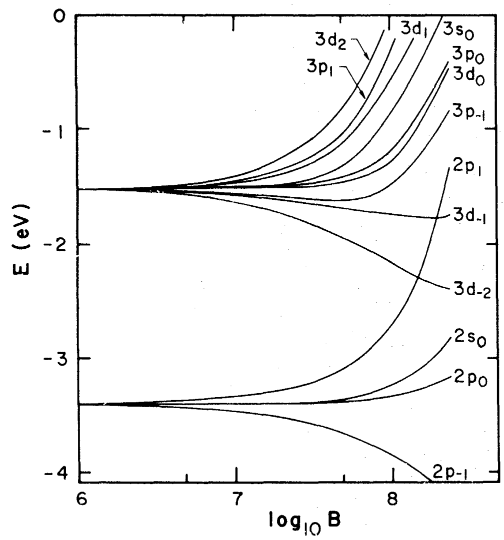

FIG. 1.—The energy spectrum of hydrogen in a magnetic field for the 13 lowest states above the ground state.

probabilities in the dipole-length approximation between all states shown in figure 1. Our results are presented in tables 1 and 2, for $B = 10^7$ and 10^8 gauss, respectively. For each transition, the first row gives the wavelength of the transition and the second row gives $A_{m'm}$ in $10^8\ \mathrm{s}^{-1}$ from equation (5).

Over the range of magnetic field strengths investigated, the transition probability increases with increasing field strength. The most dramatic increase occurs for those transitions where $\Delta n = 0$. This is due primarily to the increasing separation between the levels with larger field strength, which implies that $\omega_{m'm}$ is larger.

TABLE 1

TRANSITION PROBABILITY $A_{m'm}$ FROM EQUATION (5) FOR $B = 10^7$ GAUSS

		$2p_{-1}$	$2p_0$	$2p_1$	$3p_{-1}$	$3p_0$	$3p_1$
$1s_0$......	Wavelength	1217. Å	1210.8 Å	1203.9 Å	1025.9 Å	1021.4 Å	1016.1 Å
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	7.54(−1)*	7.49(−1)	7.46(−1)	2.03(−1)	2.01(−1)	2.01(−1)
$2s_0$......	Wavelength	21.279 μ	1258.3 μ	21.46 μ	6719.5 Å	6529.8 Å	6321.9 Å
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	2.20(−6)	1.08(−11)	2.22(−6)	2.81(−2)	2.70(−2)	2.64(−2)
$3d_{-2}$.....	Wavelength	6726.6 Å	...	...	20.590 μ	...	...
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	8.05(−2)	...	...	9.40(−6)	...	...
$3d_{-1}$.....	Wavelength	6528.9 Å	6731.9 Å	...	281.95 μ	21.373 μ	...
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	3.89(−2)	4.01(−2)	...	2.16(−9)	4.90(−6)	...
$3d_0$......	Wavelength	6341.4 Å	6532.8 Å	6741.5 Å	23.960 μ	664.40 μ	19.284 μ
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	6.81(−3)	5.22(−2)	7.24(−3)	9.14(−8)	4.87(−10)	7.36(−8)
$3s_0$......	Wavelength	6318.6 Å	6508.6 Å	6715.8 Å	21.089 μ	239.43 μ	21.657 μ
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	8.28(−3)	2.12(−3)	8.80(−3)	1.44(−5)	3.75(−9)	1.48(−5)
$3d_1$......	Wavelength	...	6332.9 Å	6528.9 Å	...	21.366 μ	281.95 μ
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	...	3.77(−2)	3.89(−2)	...	4.90(−6)	2.16(−9)
$3d_2$......	Wavelength	...	...	6328.2 Å	...	...	22.210 μ
	$A_{m'm}[10^8\ \mathrm{s}^{-1}]$	...	...	7.57(−2)	...	...	1.01(−5)

* 1.0(−1) ≡ 1.0 × 10^{-1}.

TABLE 2

TRANSITION PROBABILITY $A_{m'm}$ FROM EQUATION (5) FOR $B = 10^8$ GAUSS

		$2p_{-1}$	$2p_0$	$2p_1$	$3p_{-1}$	$3p_0$	$3p_1$
$1s_0$......	Wavelength	1267.0 Å	1204.0 Å	1132.7 Å	1019.0 Å	997.71 Å	930.31 Å
	$A_{m'm}[10^8\ s^{-1}]$	8.60(−1)*	7.82(−1)	7.69(−1)	3.16(−1)	2.43(−1)	2.88(−1)
$2s_0$......	Wavelength	2.0605 μ	13.739 μ	2.2192 μ	6968.4 Å	6079.6 Å	4217.7 Å
	$A_{m'm}[10^8\ s^{-1}]$	1.85(−3)	8.42(−6)	2.00(−3)	6.26(−2)	3.69(−2)	3.79(−2)
$3d_{-2}$.....	Wavelength	7413.5 Å	...	...	1.7499 μ	...	...
	$A_{m'm}[10^8\ s^{-1}]$	1.59(−1)	...	...	3.36(−3)	...	...
$3d_{-1}$.....	Wavelength	5905.2 Å	7807.1 Å	...	4.4066 μ	2.2897 μ	...
	$A_{m'm}[10^8\ s^{-1}]$	5.53(−2)	7.06(−2)	...	6.07(−4)	2.24(−3)	...
$3d_0$......	Wavelength	4870.5 Å	6095.1 Å	8950.5 Å	7.5728 μ	12.992 μ	1.2452 μ
	$A_{m'm}[10^8\ s^{-1}]$	5.38(−3)	6.18(−2)	9.89(−3)	2.47(−4)	6.98(−5)	4.09(−5)
$3s_0$......	Wavelength	4126.7 Å	4973.4 Å	6723.6 Å	1.9886 μ	3.4122 μ	2.3092 μ
	$A_{m'm}[10^8\ s^{-1}]$	1.48(−2)	1.14(−2)	2.41(−2)	6.15(−3)	1.47(−3)	7.14(−3)
$3d_1$......	Wavelength	...	4511.0 Å	5905.2 Å	...	2.0033 μ	4.4066 μ
	$A_{m'm}[10^8\ s^{-1}]$	...	4.08(−2)	5.53(−2)	...	1.96(−3)	6.07(−4)
$3d_2$......	Wavelength	...	...	4376.7 Å	...	...	2.7438 μ
	$A_{m'm}[10^8\ s^{-1}]$	...	...	9.36(−2)	...	...	5.26(−3)

* 1.0(−1) ≡ 1.0 × 10^{-1}.

When we include the appropriate hydrogenic wave functions, the trial solution will be exact for zero magnetic field and transition probabilities calculated in the dipole-length and dipole-momentum approximation will agree. As the field strength is increased, the representation of the wave functions will become poorer and transition probabilities calculated in the two approximations will no longer agree.

Thus, we have calculated transition probabilities in the dipole-momentum approximation as well as in the dipole-length approximation. The results are the same, to the accuracy quoted in tables 1 and 2, except for certain cases in which the energy-level separations are small. These cases, which occur only for $B = 10^8$ gauss, are displayed in table 3.

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TABLE 3

TRANSITION PROBABILITY $A_{m'm}[10^8\ s^{-1}]$ FROM EQUATIONS (3) AND (5) FOR $B = 10^8$ GAUSS, IN THE DIPOLE LENGTH (L) AND DIPOLE MOMENTUM (P) APPROXIMATION

Transition	L	P
$3d_{-1}$–$3p_0$.......	2.24(−3)	2.18(−3)
$3d_0$–$3p_{-1}$.......	2.47(−4)	2.37(−4)
$3d_0$–$3p_0$........	6.98(−5)	7.31(−5)
$3d_0$–$3p_1$........	4.09(−4)	3.92(−4)
$3s_0$–$3p_{-1}$.......	6.15(−3)	6.53(−3)
$3s_0$–$3p_0$........	1.47(−3)	1.44(−3)
$3s_0$–$3p_1$........	7.14(−3)	7.59(−3)
$3d_1$–$3p_0$........	1.96(−3)	1.90(−3)

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