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To cite this version:


HAL Id: jpa-00213866
https://hal.archives-ouvertes.fr/jpa-00213866
Submitted on 1 Jan 1970

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THE THEORY OF THE QUADRATIC ZEEMAN EFFECT

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Résumé. — Des expériences récentes à haute résolution de Garton et Tomkins ont montré des nouvelles structures dans les spectres des atomes en présence d'un champ magnétique.

On peut attribuer cesstructures au terme Hamiltonien du deuxième degré dans le champ magnétique, donnant un problème formellement inséparable. Les paramètres pertinents sont tels que les approximations ordinaires sont inefficaces.

Le but de cette étude est de surmonter ces difficultés, et les résultats préliminaires ont montré des accords encourageants avec les données.

Abstract. — Recent work at high resolution carried out at Argonne has exhibited previously unobserved structures in the spectra of atoms in magnetic fields.

These structures may be attributed to the term in the Hamiltonian quadratic in the magnetic field, giving rise to a formally non-separable problem. The relevant parameters are such that conventional approximations are invalid. The work now reported has been directed to overcoming the resulting difficulties, and preliminary results have shown promising agreement with the data.

1. Introduction. — The existence of a term in the expression for the Zeeman shift of spectral lines which is quadratic in the magnetic field has been known for many years. It was, for example, discussed by Burgers [1] in the framework of the old quantum theory. However, most textbooks — eg: Condon & Shortley [2] dismiss it as in practice a small and unimportant correction to the linear effect. In solid state physics, on the other hand, the quadratic Zeeman effect has been recognised to be of importance for some time; for even with a moderate magnetic field the frequently small effective mass of an electron in a crystal magnifies the influence of the field. (Cf.: Haideemenakis [3].)

Nevertheless, the fact that the quadratic effect is proportional to the fourth power of the principal quantum number is linked with improvements in instrumental technique to induce a new development. Long spectral series can now be resolved and the quadratic Zeeman effect can then have a major influence on spectral structure. We shall see that not only are the predictions of existing theory confirmed, but that in regions of the spectrum where n-mixing occurs spectral patterns are produced by a magnetic field, for which there is as yet no theoretical basis at all.

2. Discussion of the Results of Garton and Tomkins [5]. — These authors have published Zeeman spectra of the principal series of Ba I in absorption; the field strength was 24 070 gauss. I am grateful to Professor Garton and Dr Tomkins for information on unpublished measurements of the plates concerned.

Both the σ and π spectra may be divided into regions with strikingly different characteristics (see Fig. 1). In the lower region, running from about n = 30 to n = 37, distinct groups of lines are seen which may be identified with successive principal quantum numbers. In addition to the so-called quadratic shift, we have a breaking of the l-degeneracy characteristic of hydrogenic spectra. The lines produced are easily

![Fig. 1.](http://dx.doi.org/10.1051/jphyscol:1970411)
distinguished and have, within each group, a roughly equal spacing. The members of each group in the \( \pi \) spectrum have roughly equal intensities, while in the \( \sigma \) spectrum intensities within a group fall off rapidly, the strongest line being that with maximum displacement from the field-free position.

As we move up the series these groups start to run together and above \( n = 40 \) there is little trace of the Rydberg structure remaining. There are, however, striking regularities in the observed spectrum. In two distinct regions of the \( \sigma \) spectrum we observe sequences of regularly spaced lines, the spacing being close to \( \frac{1}{2} h\omega \), where \( \omega \) is the so-called cyclotron frequency - i.e.: \( |e| B / \mu c \). Another system of very broad lines extends from a little below the field-free series limit into the continuum. The spacing is again regular and approximately equal to \( \frac{1}{2} h\omega \). Other regularities exist, particularly in the \( \pi \) spectrum, but these are still under investigation. We may compare these evenly spaced line sequences with the so-called Landau spectrum of a free electron in a magnetic field, where the level spacing is \( h\omega \). Thus, it seems natural to call these structures \textit{quasi-Landau} levels.

The results discussed above will shortly be augmented; the use of the heat-pipe (Vidal & Cooper [9]) and the forthcoming introduction of superconducting magnets at Argonne will improve the quality of the data from Zeeman experiments still further.

3. The Theory of the Quadratic Zeeman Effect. — We shall assume in the following the complete Paschen-Back regime i.e.: that the spin of the optical electron may be ignored. This is certainly the case for the Ba I spectrum under consideration. The assumption that the effect of the nucleus and electronic core may be represented by a point charge of \( z = 1 \) is clearly also justified, provided that the quantum defects of \( p \) and possibly \( f \) orbits are taken into account. For we shall always be dealing with an optical electron with large effective principal quantum number - i.e.: with \( n > 20 \).

It is convenient to choose a vector potential

\[
A = \frac{1}{2} B \times r,
\]

where the uniform magnetic field \( B \) is along the \( z \) axis. Then, since the kinetic momentum

\[
\pi = p \dot{r} = p + \frac{|e|}{c} A
\]

(where \( p \) is the canonical momentum), the Hamiltonian for the optical electron is

\[
H = \frac{p^2}{2\mu} - \frac{|e|}{2\mu c} (p.A + A.p) + \frac{e^2}{2 \mu c^2} A^2 + U(r).
\]

The electrostatic potential

\[
U(r) = -\frac{e^2}{r} \text{ for } r \geq r_0.
\]

We shall use a frame of reference rotating with the Larmor frequency

\[
\omega = \frac{1}{2} \frac{|e| B}{\mu c}
\]

about the \( z \) axis.

In this frame the Hamiltonian becomes

\[
H^* = \frac{p^2}{2\mu} + \frac{\mu \omega^2}{8} \rho^2 + U(r) = \frac{p^2}{2\mu} + V(r)
\]

where \( \rho^2 = x^2 + y^2 \). The effective potential \( V \) is sketched in figure 2.

\[
\begin{align*}
& \text{Fig. 2.} \\
& \text{The energy of the system } E^* \text{ with respect to the Larmor frame is given by}
\end{align*}
\]

\[
E^* = E - \frac{\omega}{2} L_z,
\]

where \( E \) is the energy in the fixed frame.

The system described is non-separable, and thus there is no easy solution in either classical or quantum mechanics. It resembles in this way the well-known three-body problem.

Gajewski [4] has studied the general problem of an electron in superimposed Coulomb and magnetic fields, but his results are of limited relevance to the highly excited states characteristic of the atomic system under discussion.

Surfaces of zero velocity in the Larmor frame are given by

\[
\frac{\mu \omega^2}{8} \rho^2 + U(r) = E^*.
\]
These surfaces are sketched in figure 3 for different energies, and are the bounding surfaces of classical motion. Thus as the (negative) energy is increased, the initially spherical shape of the bounding surface becomes more and more elongated, approximating to a prolate ellipsoid. For positive energies the surface is spindle-shaped, extending to infinity along the positive and negative $z$ axes.

Although results using this approach have up to date been promising, it cannot be expected to deal adequately with that part of the spectrum where $n$ is no longer significant.

An alternative is to set up a system of coupled differential equations for the radial functions, when the wave-function of the optical electron is expanded in spherical harmonics:

$$Y_m(r, \theta, \varphi) = \sum_{l=0}^{\infty} \Phi_{lm}(r) Y_{lm}(\theta, \varphi).$$

Then the Schrödinger equation becomes

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2 \right\} \Phi_{lm}(r) =$$

$$- \frac{r^2}{4\lambda^4} \{ <lm | \sin^2 \theta | l - 2m \Phi_{lm}(r)$$

$$+ <lm | \sin^2 \theta | lm \Phi_{lm}(r)$$

$$+ <lm | \sin^2 \theta | l + 2m \Phi_{lm}(r) \} = 0$$

where

$$l = 1, 3, 5, ..., \quad k^2 = \frac{2\mu E^*}{\hbar^2}, \quad \lambda = \left[ \frac{\hbar}{m \omega} \right]^{1/2}.$$ 

Attempts are under way to produce numerical solutions of this system, although the computational problems seem formidable.

In the region around the field-free series limit ($E \approx 0$), we may expect that a legitimate approximation may be made to the solution of the quantum-mechanical problem. The semi-classical frequency of motion of the electron along the $z$ axis (proportional to $n^{-3}$) is small compared with $\omega$ and the adiabatic approximation is a natural choice. This has been considered in detail by solid state theorists. For in crystals the effective mass of an electron may be only a few per cent of the free value, so extreme cases of quadratic Zeeman effect can occur even with moderate magnetic fields (\textsuperscript{*}).

However, computations of classical orbits indicate that the adiabatic approximation must necessarily fail in the region of the origin; for here the velocity along the $z$ axis becomes large compared with the orbiting velocity. Moreover, this region is important, for we may consider it to be closely associated with radiative transitions; it is here that the selection rule against transitions other than at cyclotron frequency is broken.

Nevertheless, it is often the case in quantum theory that an unsatisfactory approximation can point to useful conclusions. A semi-classical calculation has, therefore, been made within the framework of the adiabatic approximation. In the following

\textsuperscript{*} Cf. Haidemenakis [3].
assumed close to zero, as a free parameter. We use the Bohr-Sommerfeld condition to compute the energy spectrum of an electron in a nearly plane orbit:

\[ 2^{3/2} \int_{\rho_0}^{\rho} \left[ E + \frac{e^2}{(\rho^2 + z^2)^{3/2}} - \frac{1}{2} \left( \frac{m + \mu \omega}{\hbar} \right) \right]^{3/2} \frac{1}{2} \rho^2 \frac{1}{\rho^2} \] 

\[ = \pi \hbar \left( N + \frac{1}{2} \right). \]

We seek those values of \( E \) which make \( N \) an integer. The results of numerical integration are as follows: for large \( z \), as might be expected, we get the pure Landau spectrum, with level spacing of \( \hbar \omega_0 \). As \( z \) approaches zero the uniform level spacing is preserved, at least over a range of ten levels or so. The spacing, however, increases to a limiting value of \( 1.58 \hbar \omega_0 \) in the region of \( E = 0 \). This may be compared with the experimental spacing in this region of approximately \( 1.5 \hbar \omega_0 \). Thus, the effect of the electrostatic field in inducing a higher effective orbital frequency \( \omega^{*} \) is analogous to the modification of the atomic number \( Z \) by screening in atoms and molecules.

We may use the above result along with the following argument to give a qualitative explanation of the structure of broad lines in the region of the series limit.

The motion of the electron may be regarded as having two modes: parallel to the magnetic field, and in a plane normal to the field. We associate energies \( E_\parallel \) and \( E_\perp \) with these modes. Coupling between the modes occurs through the term \( U(\rho) \).

An electron which contributes to the \( \sigma \) spectrum will have a large proportion of its energy in \( E_\parallel \). If this is greater than \( E_\perp \) for \( |z| = \infty \) it will be trapped temporarily in the magnetic bottle, although the total energy may be positive.

We see that resonances may occur, although the electron is in principle unbound. The theory underlying the width of the observed lines seems complicated and needs further work.

The picture outlined has one glaring shortcoming: at a distance about \( 5 \hbar \omega_0 \) below the series limit in the Bal \( \sigma \) spectrum, the diffuse quasi-Landau levels just dealt with start to merge with a sharply-defined quasi-Landau sequence with a spacing of about \( 4 \hbar \omega_0 \). The adiabatic hypothesis would seem to imply a gradual change of level spacing, not the observed sudden transition. The question also arises of whether the nearness of the quasi-Landau ratios to \( \frac{1}{2} \) and \( \frac{1}{3} \) is of special significance.

References