

reaction model) DWBA theory (which is first order) must sometimes fail and should be replaced by the more complete CCBA. (v) The data also show that $d_{3/2}$ and $d_{5/2}$ strength functions do not vary with A and J in the smooth way expected from giant single-particle resonance theory, apparently showing effects of substructures (doorways).

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Scaling Laws for Rydberg Atoms in Magnetic Fields

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Empirical conjectures of Feneuille, based on new regularities observed in the quasi-Landau spectrum, are investigated. Scaling laws for Rydberg atoms in magnetic fields are obtained from Schrödinger's equation, in two different approximations. Our formulas support the empirical conjectures and show them to be closely connected with the dynamics of the electronic motion in the $z=0$ plane.

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The discovery by Garton and Tomkins¹ of equally spaced resonances near the ionization limit in the absorption spectrum of barium in a magnetic field of 47 kG has greatly stimulated investigation of the properties of hydrogenic Rydberg states in a regime where Coulomb and magnetic field strengths are of comparable magnitude. The observation of regularities in this spectrum is of special relevance since the problem of such a simple atom as hydrogen in a uniform magnetic

field still remains unsolved. The basic difficulty is that the Hamiltonian for such a system is non-separable and there is no natural expansion parameter capable of adiabatically changing the spherical symmetry at vanishing magnetic field into the cylindrical symmetry of the high-field limit. A review of the problem of atoms in magnetic fields is given by Garstang² and Gay.³ Recently, the problem of hydrogenic atoms in magnetic fields has attracted much attention as a re-

sult of several experimental⁴ and theoretical^{5,6} investigations which seem to indicate that an "approximate symmetry" may exist.

In an interesting contribution Feneuille⁷ reported further regularities in the so-called quasi-Landau spectrum^{2,3} and conjectured that a scaling relation might exist, connecting the Coulomb and Landau regimes. Combining results obtained by one of us,⁸ valid for energies near the ionization limit, with results from perturbation theory,^{2,3} valid at low energies, he conjectured that the quantity n^2E might depend, in the whole energy range, only on $\beta = n^3\omega$ [n being the principal quantum number, $\omega = eB/(Mc)$ the cyclotron frequency, and B the magnetic field strength]. Fitting an equation to the experimental data of Castro *et al.*⁹ and Gay, Delande, and Biraben,¹⁰ he then suggested¹¹

$$n^2E = (\beta^2 + \frac{3}{2}\beta + \frac{9}{4})^{1/2} - (2\beta + 4)^{1/2}. \quad (1)$$

The purpose of the present communication is to report quantum scaling laws obtained by exploring the dynamics of the electronic motion along a plane perpendicular to the magnetic field. Using a recently proposed¹² procedure, we solve Schrödinger's equation in the $z=0$ plane^{2,3} and obtain a scaling law for hydrogenic atoms in uniform magnetic fields. This scaling law shows how the quantity n^2E depends on m , n , and β , where m is the magnetic quantum number of the electron. From our equations it can easily be seen that for Rydberg states ($n \gg 1$) Feneuille's empirical conjecture is a direct consequence of the motion in the $z=0$ plane. In addition, we show that a similar scaling law is predicted by the familiar two-dimensional WKB model.^{2,3}

The particular role of the dynamics in the $z=0$ plane was first recognized by Edmonds.¹³⁻¹⁶ By quantization of the electronic motion in this plane he was able to account for the striking regular spacing between the resonances measured by Garton and Tomkins¹⁻³ across the ionization limit. Meanwhile the special characteristics resulting from the motion in the $z=0$ plane have been corroborated by many people. Here we just quote the latest reports,^{6,16} from which earlier references may easily be obtained. However, we should mention the basic physical reason why motion in the $z=0$ plane is considered: It is because the so-called quasi-Landau resonances observed by Garton and Tomkins¹ and many other experimental investigators^{3,4} refer to the σ -polarization spectra (as distinct from the π spectra). For this reason, essentially all theoretical investiga-

tions start with the premise that the eigenfunction is localized in a plane perpendicular to the magnetic field, and remarkably good agreement with experiment is obtained from the Coulomb ($B \rightarrow 0$) to the Landau ($B \rightarrow \infty$) regime.^{3,4,6}

In a recent work¹² a variational technique was used to show that eigenvalues of the Schrödinger equation of a particle moving in a potential $V(r)$ may easily be obtained from the equation (we use atomic units)

$$E = \frac{1}{2}\alpha^2 + V(an/\alpha), \quad (2)$$

where a is a constant determined as in Ref. 12 and where $\alpha > 0$ is a variational parameter whose value is determined as the solution of the equation $\partial E/\partial \alpha = 0$, i.e., from

$$\alpha + (\partial/\partial \alpha)V(an/\alpha) = 0. \quad (3)$$

In the equation above we replaced the Laurent expansion $an + b + c/n + \dots$, discussed in Ref. 12, by an , which is the correct limit for Rydberg states ($n \gg 1$).

As is well known,^{2,3} the potential for the motion in the $z=0$ plane, in cylindrical coordinates, is given by^{15,16}

$$V(\rho) = -\rho^{-1} + \frac{1}{2}T\rho^{-2} + \frac{1}{8}\omega^2\rho^2, \quad (4)$$

where $T = m^2 - \frac{1}{4}$. From Eqs. (2)-(4) it is trivial to obtain

$$a^2n^2E = (\frac{1}{2} + T/2a^2n^2)x^2 - x + (a^6/8x^2)\beta^2, \quad (5a)$$

where $x \equiv an\alpha$ is the positive root of

$$(1 + T/a^2n^2)x^4 - x^3 - \frac{1}{4}a^6\beta^2 = 0. \quad (5b)$$

To obtain the eigenvalues, one first solves Eq. (5b) for the positive root,¹⁷ say x_0 ; substitution of this x_0 in Eq. (5a) then gives n^2E . Equation (5) clearly shows how n^2E depends on m^2 , n^2 , and β . As discussed in Ref. 12, $a=1$ corresponds to the pure Coulombian case ($\beta, B=0$) while $a=2$ corresponds to the pure Landau case ($\beta, B \rightarrow \infty$, the potential being a harmonic oscillator). For intermediate values of β , a is a smooth function of β bounded to the interval $1 \leq a(\beta) \leq 2$. Since the positive root x_0 is obtained from Eq. (5b), Eq. (5a) may be rewritten as

$$n^2E = a^{-2} \left[\frac{1}{2}x^2 - x + (a^6/8x^2)\beta^2 \right] \\ = (a^2x^2)^{-1} \left[\frac{1}{2}x^4 - x^3 + (\frac{1}{8}a^6)\beta^2 \right]. \quad (6a)$$

For $n \gg m$, a condition always fulfilled by Rydberg states, Eq. (5b) can be very well approximated by

$$x^4 - x^3 - (\frac{1}{4}a^6)\beta^2 = 0. \quad (6b)$$

From Eq. (6) it is seen that Feneuille's empirical expectation that n^2E is only a function of β is indeed well justified. It is interesting to observe that Eq. (6) allows one to regard the scaling as n^2E being given by a function of β [since $a=a(\beta)$] or else as a^2n^2E being given by a function of $\delta = a^3\beta$. Furthermore, because of Eq. (6b), the three-term sum in Eq. (6a) may be rewritten as

$$a^2n^2E = -\frac{1}{2}x + a^6\beta^2/4x^2 \quad (7a)$$

$$= -\frac{1}{2}x^2 + \frac{3}{8}a^6\beta^2/x^2 \quad (7b)$$

$$= x^2 - \frac{3}{2}x. \quad (7c)$$

The possibility of writing the energy as the sum of different contributions is a characteristic of separable systems. Although in the present problem we succeeded in writing the energy as a sum, the individual terms are not totally disconnected since they all depend on x . It is easy to verify that for $a=1$ ($a=2$) the scaling predicted by Eq. (6) is precisely the one obeyed by the eigenvalues of the Coulomb (harmonic oscillator) potential, as it should be. The situation for Rydberg states is privileged since only the first coefficient is needed in the Laurent expansion $an+b+c/n+\dots$. In general, the numerical values of the *truncated* Laurent expansion may depend slightly on whether one uses eigenfunctions with low or high n to obtain a, b, c, \dots . Using the same procedure described in Ref. 12, we obtained numerically the dependence $a=a(\beta)$. In the region of strongest variation, i.e., near and below the ionization limit, this dependence can, in good approximation, be taken as given by the function $a=2-e^{-0.12\beta}$. In the limit cases, for low β one has

$$n^2E \cong -\frac{1}{2} + \frac{1}{8}\beta^2,$$

and for high β

$$n^2E \cong \beta.$$

We now investigate the scaling as predicted by the familiar two-dimensional WKB model.^{2,3,13-16} As is known, the potential in Eq. (4) gives the correct spacing of the quasi-Landau resonances around $E \cong 0$ but is not simultaneously capable of reproducing the correct Landau and Coulomb limits. The Coulomb limit requires that $T_C = (|m| + \frac{1}{2})^2$, while the Landau limit imposes $T_L = m^2$. This point is discussed in more detail in Ref. 16. The WKB quantization rule is

$$\int_{\rho_1}^{\rho_2} (E + \rho^{-1} - \frac{1}{2}T\rho^{-2} - \frac{1}{8}\omega^2\rho^2)^{1/2} d\rho = (n_r + \frac{1}{2})\pi/\sqrt{2}. \quad (8)$$

Note that in Eq. (8) $n_r=0, 1, 2, \dots$ is the radial quantum number, related to the principal quantum number by¹⁶

$$n = n_r + T^{1/2} + \frac{1}{2}. \quad (9)$$

A simple change of variable [$y \equiv \rho/n^2$] in Eq. (8) gives

$$\int_{y_1}^{y_2} \left(n^2E + \frac{1}{y} - \frac{T}{2n^2y^2} - \frac{1}{8}\beta^2y^2 \right)^{1/2} dy = \frac{(n_r + \frac{1}{2})\pi/\sqrt{2}}{n_r + T^{1/2} + \frac{1}{2}}. \quad (10)$$

For Rydberg states the right-hand side of Eq. (10) is approximately $\pi/\sqrt{2}$. The integral in this equation can be analytically evaluated in terms of complete elliptic integrals.¹⁶ For $T=0$ or $n \gg 1$ it follows directly from inspection of Eq. (10) that n^2E only depends on β . When $T \neq 0$ the m dependence of Eq. (10) arises from the $T/2n^2$ term, i.e., we have an m^2/n^2 term exactly as in Eq. (5). The WKB model provides an implicit equation for the scaling, while our previous approach provides a more explicit one.

In Fig. 1 we compare the scalings for n^2E as given (i) by Eq. (10) with $n=n_C=n_r+T^{1/2}+\frac{1}{2}$, $m=0$, and $T=T_C=\frac{1}{4}$, (ii) by Eq. (1), according to Feneuille, and (iii) by Eq. (6). This figure shows the energy region near the ionization threshold ($E \cong 0$) and below it. This region has been extensively studied by experimentalists and coincides with the region where the scaling n^2E has its strongest variation. As is readily seen from the figure, the agreement between the three scaling laws is quite good. The region around the ionization threshold is shown in more detail in Fig. 1(b). The relative difference between the scaling as predicted by the two-dimensional WKB model and Feneuille's relation [our Eq. (1)] is noteworthy. The two-dimensional model has been reported by several experimental groups as reproducing the measured data well, while Feneuille's relation was obtained through a direct fit of recent high-resolution observations. In particular, Feneuille's relation and our Eq. (6) predict $n^2E \cong 0$ at $\beta_0 \cong 1.6$, while the WKB model predicts $\beta_0 \cong 1.56$. Because of the slight m dependence in Eqs. (5) and (10), we do not expect β_0 to change significantly with m . Clearly, a detailed experimental investigation of these equations would be of much interest.

In summary, we believe that Feneuille's conjecture that n^2E scales as a function of β is more than a conjecture. We consider this new regular-

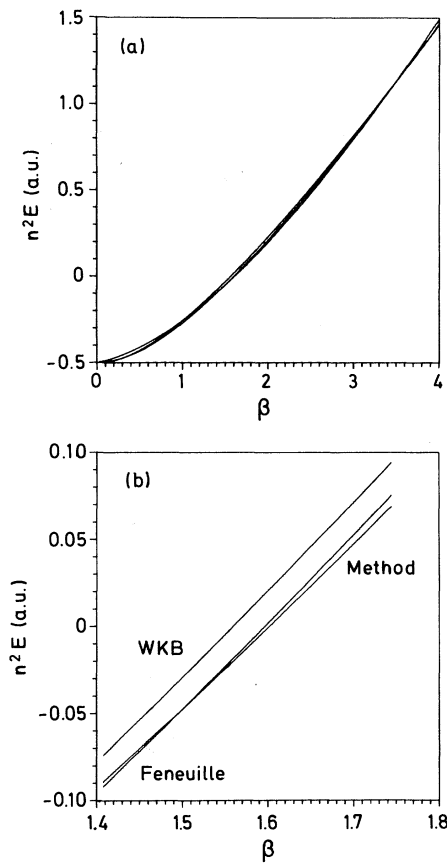


FIG. 1. The quantity $n^2 E$ vs $\beta = n^3 \omega$ as predicted by the three scaling formulas discussed in the text: Eq. (10), "WKB"; Eq. (1), "Feneuille"; and Eq. (6), "Method." (a) The Coulomb to Landau regime. The small percentage difference between the three formulas is barely noticeable. (b) Detail around the ionization threshold (see text).

ity in the quasi-Landau spectrum to be closely connected with dynamic properties of the electronic motion along the $z=0$ plane. We have further investigated how the m quantum number would influence the scaling and found the influence to be negligible. As a last remark we observe that although in the present work we concentrated on the scaling of the quasi-Landau resonances, the equations discussed here have a number of other applications.^{2,3} As one example we quote the study of hydrogenic excitons in magnetic fields.¹⁸

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