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LETTER TO THE EDITOR

On the scaling properties of the energy spectrum of hydrogen in a uniform magnetic field

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Abstract. The magnetic-field scaling relation between the coordinates, momenta and the energy in the Hamiltonian for the Kepler motion in a uniform magnetic field, i.e.

$$H(\gamma^{-1/3}p, \gamma^{2/3}r; \gamma^{1/3}m, \gamma=1) = \gamma^{-2/3}H(p, r; m, \gamma),$$

where $\gamma = B/B_0$ is the normalised field strength and m the constant value of the angular momentum B-parallel component, is shown to ensure a representation of the semiclassical energy spectrum: $E = (n+\frac{1}{2})^{-2}f(\gamma^{1/3}(n+\frac{1}{2}), \gamma^{1/3}m)$, $m = 0, \pm 1, \ldots; n = 0, 1, \ldots$. We discuss how the function f, in the two-dimensional approximation ($z = p_z = 0$, $z//B$), can be constructed.

In computing quantal energy levels, several authors have utilised various scaling properties found in the (classical) Hamiltonian function for the hydrogen-like atom in presence of a uniform magnetic field B; namely, that in terms of the nuclear charge (Surmelian and O'Connell 1974), of a mass ratio (Wunner and Ruder 1982) and of the B-parallel component of the angular momentum (Robnik 1981) (this is for computing the onset critical energy of irregular motions). Among such, it should be of great value for direct information about the quantal energy spectrum, if the scaling of the energy as a function of the action variables can be established. The reason is obviously that it provides a possible structure in representing the semiclassical energy eigenvalue against the quantum number that is related to a fixed action variable, if well defined.

In their analyses of experiments, Fonck *et al* (1980) noted that the WKB quantising condition for the two-dimensional approximation to the above systems (i.e. $p_z = z = 0$, $z//B$, in the Hamiltonian) can be expressed as a field-free form, if the energy and the action variable (or, the quantum number) are multiplied by $B^{-2/3}$ and $B^{1/3}$, respectively, for the special case $L_z = m = 0$ (the angular momentum z-component vanishes). This fact is equivalent to saying that the energy is given by a single function of the field, if the former is scaled by n^{-2} and the latter by n^{-3} where n represents the quantum number of the semiclassical quantisation, as pointed out by Feneuille (1982) who expressed the relation as

$$\varepsilon = f(\beta); \qquad \varepsilon = n^2 E, \qquad \beta = n^3 B. \tag{1}$$

This form of stating the scaling law for the (two-dimensional) magnetised hydrogen atom, hereafter called Feneuille's form, seems to bear a fundamental significance because the field involved is entirely arbitrary in strength. For example, it unifies the convenient argument of both strong- and weak-field regimes by Rau (1977), and it predicts a straight line of the plot n against $B^{-1/3}$ at the ionisation threshold $E=0$, which has been experimentally verified (Gay *et al* 1980, Delande *et al* 1982).

This letter presents our consideration that (1) can be extended to the case of non-vanishing value of $L_z=m$ in the form

$$(n+\tfrac{1}{2})^2E=f(\gamma(n+\tfrac{1}{2})^3,\ \gamma m^3), \tag{2}$$

$$\gamma=B/B_0=\tfrac{1}{2}\hbar\omega/\mathrm{Ry}\ \text{(the normalised field strength)}, \tag{2a}$$

i.e. for the general value of L_z there exists a function of two variables such that, with the same cubic scaling of both quantum numbers $n(=0,1,2\ldots)$ and $m(=0,\pm1,\pm2\ldots)$, Feneuille's form (1) can still be valid (the replacement of n by a half integer is due to the well known reason of the WKB procedure for 'vibrations'). We argue that the generalised form (2) can be deduced from a certain scaling relation satisfied in the Hamiltonian for the Kepler motion in a magnetic field, where the function f can be constructed, at least within the two-dimensional approach, in terms of a set of parameter representations of the E against γ relation†.

Let H denote the Hamiltonian for a charged particle with unit mass under the combined action of uniform magnetic and fixed Coulomb fields, indicating it as a function of the canonical variables of the momentum vector p and the coordinate r together with the two parameters γ and m; $H(p,r;m,\gamma)$ is given by

$$H(p,r;m,\gamma)=\tfrac{1}{2}(p+(e/2c)B\times r)^2-e^2/r \tag{3a}$$

$$=\tfrac{1}{2}(p_\rho^2+p_z^2)+L_z^2/2\rho^2+\tfrac{1}{8}\omega^2\rho^2-e^2/(\rho^2+z^2)^{1/2}+\tfrac{1}{2}\omega L_z \tag{3b}$$

(ω is the cyclotron frequency) with

$$m=L_z/\hbar, \qquad \gamma=\hbar\omega/2\mathrm{Ry}. \tag{3c}$$

Then it is easy to see that the following relation holds:

$$H(\gamma^{-1/3}p,\gamma^{2/3}r;\gamma^{1/3}m,\gamma=1)=\gamma^{-2/3}H(p,r;m,\gamma). \tag{4}$$

This is the unified form of the two scaling relations previously noted for $m\neq0$ (Robnik 1982, Harada and Hasegawa 1983), and may be considered as fundamental and generic to the diamagnetism of atoms.

Suppose that the classical equations of motion with Hamiltonian (3) allow a set of trajectories that form an invariant torus located in a hypersurface of $H=E$ and $L_z=m$. It may be considered as embedded in the four-dimensional phase space $(p_\rho,\rho;p_z,z)$ with fixed m (see (3b)) and with the topology of the two-dimensional two-torus. Since the Hamiltonian is non-separable, such a situation may occur in restricted ranges of the constants E and m, i.e. in an approximately integrable region for the constant hypersurfaces (called a 'remnant', see Reinhardt and Farrelly (1982)). Then, two independent action variables J_1 and J_2 should be well defined by $\int_{C_i}p\,\mathrm{d}r$ ($i=1,2$) with closed integration contours C_1 and C_2 that are topologically distinct but each continuously deformable without changing the integrals on the torus. What is the significance of the fundamental scaling relation (4), when applied to these action variables?

The answer to this question can be written down by specifying the two action variables as functions of E and Λ (Λ denotes an unknown variable to specify, together with E, the two-dimensional torus) as well as of the parameters m and γ; $J_i(E,\Lambda;m,\gamma)$.

† See our note added at the end about the recent paper by Gallas *et al* (1983).

Since the action variable J_i represents the area inside the contour C_i, the scaling $p \to \gamma^{-1/3}p$, $r \to \gamma^{2/3}r$ implies that $J_i \to \gamma^{1/3}J_i$; thence

$$\gamma^{-1/3}J_i(\gamma^{-2/3}E, \Lambda_\gamma; \gamma^{1/3}m, 1) = J_i(E, \Lambda; m, \gamma), \qquad i = 1, 2. \tag{5}$$

Or, by considering the inverse function of $J_1(E, \Lambda)$ and $J_2(E, \Lambda)$ with parameters m and γ being fixed, we get

$$\gamma^{2/3}E(\gamma^{1/3}J_1, \gamma^{1/3}J_2; \gamma^{1/3}m, 1) = E(J_1, J_2; m, \gamma). \tag{6}$$

Note that the result is irrespective of the γ scaling of the unknown variable Λ indicated as Λ_γ in (5). Let us fix our attention on the first action variable $J_1 \equiv J$ whose periodicity of motion is assumed as 'vibration like' (as contrasted to the rotation-like periodicity for m), and forget about the second one J_2. The desired representation of the quantised energy

$$E = (n+\tfrac{1}{2})^{-2} f(\gamma^{1/3}(n+\tfrac{1}{2}), \gamma^{1/3}m) \tag{7}$$

is a consequence of the EBK quantisation (Percival 1977)

$$J = \int_{C_1} p \, \mathrm{d}r = (n+\tfrac{1}{2})h \tag{8}$$

and of defining the function $f(J, m)$ by

$$f(J, m) \equiv (J/h)^2 E(J/h; m, \gamma = 1). \tag{9}$$

Feneuille's form (2) may be obtained by an appropriate redefinition of the variables in f in the above. We also note that the full knowledge about $J_i(E, \Lambda; m, \gamma)$, $i = 1, 2$, provides us with the complete representation in terms of the three sets of quantum numbers (n, k, m) in the form

$$E = (n+\tfrac{1}{2})^{-2} f(\gamma^{1/3}(n+\tfrac{1}{2}), \gamma^{1/3}(k+\alpha/4), \gamma^{1/3}m).$$

Thus, the problem of quantising the hydrogen atom in a magnetic field of arbitrary strength (in a semiclassical version) reduces to determination of the two action variables on the invariant torus, as far as it exists, for one particular value of the field (e.g. $\gamma = 1$) but as functions of E, Λ and m. Here, we discuss a more detailed procedure of constructing the function f in (7) under the approximation of $z = p_z = 0$ in (3*b*) of the Hamiltonian in the cylindrical coordinates sytem. This makes the problem effectively one-dimensional, and has been used for investigation of the *quasi-Landau resonances* QLR (Edmonds 1970, Starace 1973, Gallas and O'Connell 1982a, b) in terms of the explicit form of $J(E; m, \gamma)$:

$$J = 2^{3/2} \int_{\rho_1}^{\rho_2} \left(E' - \frac{(\hbar m)^2}{2\rho^2} + \frac{e^2}{\rho} - \frac{\omega^2}{8}\rho^2 \right)^{1/2} \mathrm{d}\rho, \qquad E' = E - \frac{\hbar\omega}{2}m, \tag{10}$$

where $\rho_{1,2}$ ($\rho_1 \leqslant \rho_2$) are the two real positive roots of the square root.

It is necessary to invert the function $J = J(E; m, \gamma)$ with respect to E for the representation (7) and we will show that this can be facilitated by a set of parameter representations. The problem for the special case $m = 0$ was solved by Akimoto and Hasegawa (1967) before the discovery of QLR: there exist two functions of a parameter u, $F(u)$ and $G(u)$ through which

$$\gamma = F(u)/(n+\tfrac{1}{2})^3 \qquad \text{and} \qquad E = G(u)/(n+\tfrac{1}{2})^2. \tag{11}$$

This implies automatically the validity of Feneuille's form, and therefore

$$E = (n+\tfrac{1}{2})^{-2} f(\gamma^{1/3}(n+\tfrac{1}{2})) \qquad (m=0 \text{ in } (7))$$

with $f(x) = G(\{F^{-1}(x)\}^{1/3})$.

The notation u for the parameter in the representation (11) is different from the original one in Akimoto and Hasegawa (1967). These authors discussed how the analytic representation (11) can be used to study the γ dependence of the energy spectrum: for example, the weak-field and strong-field behaviours can be correctly derived. (In Gallas and O'Connell (1982a), an incorrect formula has been pointed out for $\mathrm{d}E/\mathrm{d}n$ expressed in terms of the complete elliptic integrals in the above paper. This is due to the complexity of transformation into the standard form of the elliptic integrals given in the appendix. We note that there is nothing wrong in the main part of Akimoto–Hasegawa, which we have reconfirmed.) Here, for future purposes we present an account of how to derive (11) without recourse to the use of elliptic functions.

Following Gallas and O'Connell (1982a), we factor the inside of the square root of the integrand in (10), so that for $m=0$

$$-\rho^3 + 8E\rho/\omega^2 + 8e^2/\omega^2 \equiv (\rho_0 - \rho)[(\rho-b)^2 + a^2], \tag{12a}$$

from which

$$b = -\tfrac{1}{2}\rho_0 \qquad \text{and} \qquad a^2 + \tfrac{1}{4}\rho_0^2 = (8e^2/\omega^2)\rho_0^{-1}, \tag{12b}$$

$$a^2 - \tfrac{3}{4}\rho_0^2 = -8E/\omega^2. \tag{12c}$$

Equations (12*b*) and (12*c*) are combined to give

$$E = \frac{2a_\mathrm{B}}{\rho_0}\left[\left(\frac{\rho_0}{2a_\mathrm{B}}\right)^3 \gamma^2 - 1\right]\mathrm{Ry} \qquad (a_\mathrm{B}\text{: Bohr radius, Ry: Rydberg energy}). \tag{12d}$$

Then the parameter u may be introduced as

$$u = (\rho_0/2a_\mathrm{B})^3 \gamma^2, \tag{13}$$

so that the u representation (11) is available, if the classical turning distance ρ_0 can be eliminated from

$$E = (2a_\mathrm{B}/\rho_0)(u-1)\mathrm{Ry}, \qquad \gamma = (2a_\mathrm{B}/\rho_0)^{3/2} u^{1/2}. \tag{14}$$

But this is possible by rearranging the integral for J:

$$J = 2\int_0^{\rho_0} [2(E - V(\rho))]^{1/2}\,\mathrm{d}\rho = \left(\frac{\rho_0}{2a_\mathrm{B}}\right)^{1/2} 4\hbar \int_0^1 \left(\frac{1-x}{x}[u(x+x^2)+1]\right)^{1/2} \mathrm{d}x. \tag{15}$$

Thus, we can set

$$\left(\frac{2a_\mathrm{B}}{\rho_0}\right)^{1/2} = \frac{h}{J}\Phi(u), \qquad \Phi(u) \equiv \frac{2}{\pi}\int_0^1 \left(\frac{1-x}{x}[u(x+x^2)+1]\right)^{1/2} \mathrm{d}x \tag{16}$$

obtaining

$$\gamma = (n+\tfrac{1}{2})^{-3} u^{1/2}\{\Phi(u)\}^3, \qquad E = \frac{\mathrm{Ry}}{(n+\frac{1}{2})^2}(u-1)\{\Phi(u)\}^2. \tag{17}$$

These indicate, in (11) in terms of $\Phi(u)$ given by (16),

$$F(u)=u^{1/2}\{\Phi(u)\}^3 \qquad \text{and} \qquad G(u)=(u-1)\{\Phi(u)\}^2\text{Ry}. \tag{18}$$

It may be remarked here that the plausibility of the half-integer quantum number for the above case of $m=0$ (absence of the centrifugal potential) can be assured from a more detailed analysis of the wavefunction near the turning point $\rho=\rho_0$ as well as $\rho=0$, as discussed in Akimoto and Hasegawa (1967).

We briefly summarise a feature of the representation (17). The function $\Phi(u)$ defined by (16) is smoothly varying for $0\leqslant u<\infty$, with $\Phi(0)=(2/\pi)\int_0^1(1-x)^{1/2}x^{-1/2}\,dx=1$, $\Phi(4)=(4/\pi)\int_0^1(1-x)^{1/2}x^{-1/2}(\frac{1}{2}+x)\,dx=\frac{3}{2}$, and $\Phi(u\gg 1)\sim\frac{1}{2}u^{1/2}+\pi^{-1}u^{-1/2}\log u$ (asymptotic expansion). Thus, the field variation $\gamma=0\to\infty$ corresponds to the u variation $u=0\to\infty$, and from (17) the negative energy-range is represented by the interval $u\in[0,1]$, where $\Phi(u)$ changes only slightly:

$$\Phi(0)=1\to\Phi(u)=1+\tfrac{3}{16}u+\ldots\to\Phi(1)=(2/3\pi)B(\tfrac{3}{2},\tfrac{1}{6})$$

$$=1.159\ldots \qquad (B(.,.)\text{: the beta function}). \tag{19}$$

The power series expansion (19) yields the low-field regime (quadratic Zeeman regime), while the asymptotic expansion of $\Phi(u)$ for $u\gg 1$ yields the quasi-Landau regime in the sense of Rau (1977), as shown in table 1.

Table 1. The low-field and high-field expressions of the energy derived by a power-series and an asymptotic expansion of $\Phi(u)$, (16).

$0<u<1$	$1\ll u$
$\Phi(u)=1+\frac{3}{16}u$	$\Phi(u)\sim\frac{1}{2}u^{1/2}(1+(2/\pi)u^{-1}\log u)$
$F(u)=u^{1/2}(1+\frac{9}{16}u)$	$F(u)\sim\frac{1}{8}u^2(1+(6/\pi)u^{-1}\log u)$
$G(u)=-1+\frac{5}{8}u$	$G(u)\sim\frac{1}{4}u^2$
$E=-(n+\frac{1}{2})^{-2}+\frac{5}{8}(n+\frac{1}{2})^4\gamma^2$	$E=\gamma(2n+1)-C^*(\gamma/(2n+1))^{1/2}$ (energy in unit of Ry)

† $C=(6/\pi)C_0$, where C_0 is appropriately chosen to replace $\log u$.

Feneuille (1982) noted that the existence of the single function $f(\beta)$ for the scaled energy-field relation provides two formulae for mean values: these are, in the two-dimensional approach, given by

$$\langle\rho\rangle^{-1}=(2/n^2)(\beta\,\mathrm{d}f/\mathrm{d}\beta-f(\beta)), \qquad \langle\rho^2\rangle=(4n^4/\beta)\,\mathrm{d}f/\mathrm{d}\beta, \tag{20}$$

where

$$\langle A\rangle\equiv\int_0^{\rho_0}\frac{A(\rho)\,\mathrm{d}\rho}{[2^{-1}(E-V(\rho))]^{1/2}}\Bigg/\int_0^{\rho_0}\frac{\mathrm{d}\rho}{[2^{-1}(E-V(\rho))]^{1/2}}. \tag{21}$$

We have ascertained them in detail, and obtained a further reduction in terms of our parameter representation as follows:

$$\left\langle\frac{1}{\rho}\right\rangle=\frac{2\{\Phi(u)\}^2}{(n+\frac{1}{2})^2}\frac{(1+u)\Phi(u)+2(u-u^2)\Phi'(u)}{\Phi(u)+6u\Phi'(u)} \tag{22a}$$

$$\langle\rho^2\rangle=\frac{8(n+\frac{1}{2})^4}{\{\Phi(u)\}^4}\frac{\Phi(u)-2(1-u)\Phi'(u)}{\Phi(u)+6u\Phi'(u)} \qquad \text{(length in units of } a_{\mathrm{B}}). \tag{22b}$$

Finally, let us discuss how the parameter representation (17) can be extended to the general case of $m \neq 0$. The procedure of factoring the square-root in the WKB integrand for $m = 0$ suggests that it can be done by setting (Gallas and O'Connell 1982b)

$$-\rho^4 + \frac{8E'}{\omega^2}\rho^2 - \frac{8e^2}{\omega^2}\rho + \frac{4(m\hbar)^2}{\omega^2} = (\rho_2 - \rho)(\rho - \rho_1)[(\rho - b)^2 + a^2], \qquad \rho_1 < \rho_2. \tag{23}$$

Clearly, the lower turning point ρ_1 tends to 0 for the limit $m \to 0$ (see figure 1), and here let us define

$$\rho_0 \equiv \rho_1 + \rho_2. \tag{24}$$

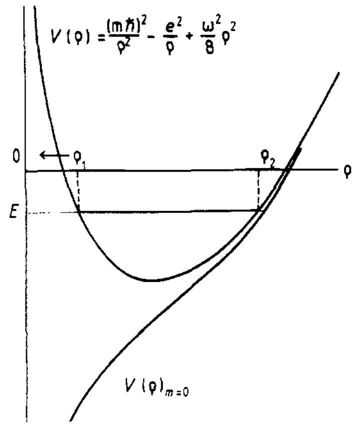

Figure 1. The potential function $V(\rho)$ in the cylindrical coordinate system of the two-dimensional hydrogen atom; for $m \neq 0$ (presence of the centrifugal part) and the limit $m \to 0$.

Then, the introduction of the parameter u in (13) still works by replacing (12*b*) and (12*c*) by

$$a^2 + \tfrac{1}{4}\rho_0^2 = 4(m\hbar)^2/\omega^2\rho_1\rho_2 \tag{25a}$$

$$= (8e^2/\omega^2)\rho_0^{-1} + \rho_1\rho_2, \tag{25b}$$

$$a^2 - \tfrac{3}{4}\rho_0^2 = 8E'/\omega^2 - p_1\rho_2. \tag{25c}$$

Here, one more parameter is needed, for which we define

$$v \equiv \rho_1/(\rho_1 + \rho_2) \qquad \text{and so } 1 - v = \rho_2/(\rho_1 + \rho_2). \tag{26}$$

The condition $\rho_1 < \rho_2$ implies

$$0 < v < \tfrac{1}{2}. \tag{27}$$

The WKB integral (15) now becomes

$$J = 2\int_{\rho_1}^{\rho_2} [2(E' - V(\rho))]^{1/2}\,d\rho$$

$$= \left(\frac{\rho_0}{2a_B}\right)^{1/2} 4\hbar \int_v^{1-v} \{(1 - v - x)(x - v)[u(x + x^2) + uv(1 - v) + 1]\}^{1/2} \frac{dx}{x}.$$

Consequently, by defining

$$\Phi(u, v) \equiv \frac{2}{\pi} \int_v^{1-v} \{(1-v-x)(x-v)[u(x+x^2)+uv(1-v)+1]\}^{1/2} \frac{dx}{x}, \tag{28}$$

we obtain the uv representation as follows:

$$\gamma = \frac{\Phi^3}{(n+\frac{1}{2})^3} u^{1/2}, \qquad E' = \frac{\Phi^2}{(n+\frac{1}{2})^2}(u-1-2uv(1-v)) \text{ Ry},$$
$$\gamma^{1/3} m = u^{1/6}[4v(1-v)(uv(1-v)+1)]^{1/2} \equiv \mu. \tag{29}$$

The last relation indicates that v is solvable in terms of u and μ through

$$v(1-v) = (2u)^{-1}[-1+(1+\mu^2 u^{2/3})^{1/2}], \tag{30}$$

and therefore by denoting $\Phi_\mu(u) \equiv \Phi(u, v(u, \mu))$

$$\gamma = \frac{\{\Phi_\mu(u)\}^3}{(n+\frac{1}{2})^3} u^{1/2}, \qquad E' = \frac{\{\Phi_\mu(u)\}^2}{(n+\frac{1}{2})^2}[u-(1+\mu^2 u^{2/3})^{1/2}]. \tag{31}$$

Thus, it generalises the representation (17) for $m = 0$ to $m \neq 0$, verifying directly the form (7) by virtue of (29).

Very recently, Gallas *et al* (1983) have presented a discussion of Feneuille's scaling law based on their own approach to solving the pertinent Schrödinger equation as well as on the WKB integral (10) in their belief that the law is more than a conjecture. We emphasise here that the law stems from the most accurate scaling relation (4) together with the EBK quantisation (8) so that its validity is not restricted to the two-dimensional model, and that our procedure of the parameter representation for the model proves the validity explicitly.

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