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**LETTER TO THE EDITOR**

# Two-dimensional quantisation of the quasi-Landau hydrogenic spectrum

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**Abstract.** Based on the two-dimensional WKB model, an equation is derived from which the non-relativistic quasi-Landau energy spectrum of hydrogen-like atoms may be easily obtained. In addition, we discuss the solution of radial equations in the WKB approximation and its relation with models recently used to fit experimental data.

The two-dimensional WKB model (Edmonds 1970, Starace 1973, Garstang 1977) has been very useful in the interpretation of experimental data concerning the quasi-Landau spectrum of hydrogen-like atoms. Although it is relatively crude, the success of the model is evident from work published in recent years (Fonck *et al* 1978, 1980, Economou *et al* 1978, Castro *et al* 1980, Gay *et al* 1980, Delande and Gay 1981a, b, Kara and McDowell 1981, Clark and Taylor 1980, 1982, Ferrante *et al* 1982). The model consists basically of studying the complicated motion of a spinless particle of mass $M$ in combined Coulomb and magnetic fields through the central potential

$$V(\rho) = -\frac{qt}{\rho} + \frac{rt}{\rho^2} + t\rho^2 \tag{1}$$

where $r \geqslant 0$ and $q$ and $t$ are positive quantities. More specifically, $t = M\omega^2/8$, $q = e^2/t$ and $r = \hbar^2 T/2Mt$, where $\omega = eB/Mc$ is the cyclotron frequency and $T$ is a known function of the magnetic quantum number $m$. The notation of the present work is consistent with that of Gallas and O'Connell (1982a, b); for further details see the review article of Garstang (1977) and the recent work of Gay (1980) and Rau (1980).

In some of the previously mentioned works (Fonck *et al* 1978, 1980, Economou *et al* 1978, Gay *et al* 1980, Delande and Gay 1981a, b) the quasi-Landau spectrum was obtained *numerically* from the first-order WKB quantisation rule, namely from the equation

$$I = \int_{\rho_1}^{\rho_2} \frac{d\rho}{\rho} (-\rho^4 + p\rho^2 + q\rho - r)^{1/2} = (n + \tfrac{1}{2}) \frac{\pi\hbar}{(2Mt)^{1/2}} = (n + \tfrac{1}{2}) \frac{2\pi\hbar}{M\omega} \tag{2}$$

where $p = (E - \frac{1}{2}m\hbar\omega)/t$, $E$ being the energy of the electron, and $\rho_1 < \rho_2$ the two real and non-negative roots of

$$-\rho^4 + p\rho^2 + q\rho - r \equiv (\rho - \rho_1)(\rho_2 - \rho)(\rho^2 - 2X\rho + Y) = 0. \tag{3}$$

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In the present letter we show that the integral in equation (2) can be analytically evaluated giving a transcendental equation, in terms of complete elliptic integrals, from which the quantised spectrum may be easily obtained.

We proceed by introducing the convenient definition

$$I_j = \int_{\rho_1}^{\rho_2} \rho^j(-\rho^4 + p\rho^2 + q\rho - r)^{-1/2}\,\mathrm{d}\rho \tag{4}$$

which allows the integral in equation (2) to be written as

$$I = -I_3 + pI_1 + qI_0 - rI_{-1}. \tag{5}$$

Furthermore, from the identity

$$\int_{\rho_1}^{\rho_2} (E - V(\rho))^{1/2}\,\mathrm{d}\rho = \tfrac{1}{2}\int_{\rho_1}^{\rho_2} \frac{\rho V'(\rho)}{(E - V(\rho))^{1/2}}\,\mathrm{d}\rho \tag{6}$$

which is obtained by a trivial integration by parts of the left-hand side of equation (6), it follows that

$$I = I_3 + \tfrac{1}{2}qI_0 - rI_{-1} \tag{7}$$

Combining equations (5) and (7), we therefore obtain

$$I = \tfrac{1}{2}pI_1 + \tfrac{3}{4}qI_0 - rI_{-1}. \tag{8}$$

The analytical evaluation of $I_1$, $I_0$ and $I_{-1}$ depends on the quadratic polynomial in equation (3). For physically meaningful energies such that the discriminant $D = X^2 - Y \leqslant 0$ (or equivalently, for energies $E \leqslant V_c$ where $V_c$ is the relative minimum of $V(\rho)$ in the negative $\rho$ axis (see Gallas and O'Connell 1982b)) one has

$$\rho^2 - 2X\rho + Y \equiv (\rho - b)^2 + a^2.$$

Calling

$$A^2 = (\rho_2 - b)^2 + a^2 \qquad B^2 = (\rho_1 - b)^2 + a^2 \qquad \text{and} \qquad k^2 = [(\rho_1 - \rho_2)^2 - (A - B)^2]/4AB$$

we find

$$I_0 = 2g\mathbf{K}(k) \tag{9}$$

$$I_1 = \frac{g}{A - B}[2(\rho_1 A - \rho_2 B)\mathbf{K}(k) + (A + B)(\rho_2 - \rho_1)\mathbf{\Pi}(\alpha_1^2, k)] \tag{10}$$

$$I_{-1} = \frac{g}{\rho_1\rho_2(\rho_1 A - \rho_2 B)}[2\rho_1\rho_2(A - B)\mathbf{K}(k) + (\rho_1 - \rho_2)(\rho_1 A + \rho_2 B)\mathbf{\Pi}(\alpha_2^2, k)] \tag{11}$$

where

$$g = (AB)^{-1/2} \qquad \alpha_1^2 = -(A - B)^2/4AB \qquad \alpha_2^2 = -(\rho_1 A - \rho_2 B)^2/4\rho_1\rho_2 AB$$

and $\mathbf{K}(k)$ and $\mathbf{\Pi}(\alpha^2, k)$ are the complete elliptic integrals of the first and third kinds, respectively (Byrd and Friedman 1975). For $D > 0$ $(E > V_c)$ $\rho^2 - 2X\rho + Y \equiv (\rho - c)(\rho - d)$ and it follows (assuming $d < c < 0$)

$$I_0 = g\mathbf{K}(k) \tag{12}$$

$$I_1 = g\left[d\mathbf{K}(k) + (\rho_2 - d)\mathbf{\Pi}\left(\frac{\rho_1 - \rho_2}{\rho_1 - d}, k\right)\right] \tag{13}$$

$$I_{-1}=\frac{g}{\rho_2 d}\left[\rho_2\mathbf{K}(k)+(d-\rho_2)\mathbf{\Pi}\left(\frac{d(\rho_1-\rho_2)}{\rho_2(\rho_1-d)},k\right)\right] \tag{14}$$

where now

$$g=2/[(\rho_1-d)(\rho_2-c)]^{1/2} \qquad \text{and} \qquad k^2=[(\rho_2-\rho_1)(c-d)]/[(\rho_1-d)(\rho_2-c)].$$

Observe that the spacing between the quasi-Landau resonances is given by $dE/dn = \pi\hbar\omega/(2I_1)$.

From the equations above one sees that the numerical evaluation of $I$ is reduced to the evaluation of just $\mathbf{K}(k)$ and $\mathbf{\Pi}(\alpha^2, k)$. This is indeed a trivial task and, with existing algorithms (e.g. Carlson 1979), may be easily performed even on a programmable pocket calculator. For the case $r=0$ (corresponding to $T=0$) one finds $\rho_1=0$ and, therefore, $I_{-1}$ need not be evaluated since the last term on the right-hand-side of equation (8) vanishes. For the particular case $r=0$ we observe that Akimoto and Hasegawa (1967) also evaluated the integral $I$. However, their results do not agree with ours. In fact, we have previously shown that their results for the spacing are incorrect (Gallas and O'Connell 1982a). The correctness of our equations was checked by numerically integrating $I_1$, $I_0$ and $I_{-1}$ for non-trivial values of $p$, $q$ and $r$.

While evaluating the analytical expressions it was noted that the *de facto* condition for the validity of equations (9)–(11) is $A^2>0$ and $B^2>0$ rather than $D\leqslant 0$, as claimed in the handbook of elliptic integrals (Byrd and Friedman 1975). This allows one to use the integrals well out of the intervals defined by Byrd and Friedman.

Before proceeding we would like to discuss briefly the solution of radial equations in the WKB approximation. It is well known, though not widely so, that when applying the WKB approximation to radial equations some care is needed. As pointed out by Langer (1937), the quantisation condition for one-dimensional problems is derived under the assumption that the eigenfunctions go to zero as one approaches $\pm\infty$. For a radial equation, on the other hand, the solutions approach zero for $r\to 0$ and $r\to\infty$. Therefore, if one wants to apply the one-dimensional WKB quantisation rule, derived for $-\infty<x<\infty$, to a radial problem, defined in $0\leqslant r<\infty$, one should map the semi-infinite into an infinite interval. To this end Langer used the mapping $x=\ln r$. The effect of the mapping is to introduce corrections $\Delta V$ in the potential. In this way one easily obtains the celebrated correction $l(l+1)/r^2\to l(l+1)/r^2+1/4r^2=(l+\frac{1}{2})^2/r^2$ for the hydrogen atom. However, it is clear that the choice of the mapping function is arbitrary. Unfortunately, as shown by Adams and Miller (1977), different choices of mapping function produce different corrections $\Delta V$. This means that by properly choosing the mapping one could, in principle, perform any desired 'correction' $\Delta V$ to the potential. One way out of the dilemma is the Adams–Miller conjecture: the mapping function, and therefore the correction $\Delta V$, should be chosen such that the correct quantum mechanical result is obtained if the potential $V$ is set to zero. For the semi-infinite interval this criterion selects the Langer transformation $x=\ln r$ uniquely. By Langer-transforming the radial equation with the potential of equation (1), one sees that the WKB approximation requires $T=m^2$. This was the choice of Akimoto and Hasegawa (1967) and of Fonck *et al* (1980). In the absence of the ionic core, i.e. for $q=0$ in equation (1), it is easy to verify that the eigen-energies from equation (2) are precisely the spinless Landau levels:

$$E=[n+\tfrac{1}{2}(m+|m|+1)]\hbar\omega. \tag{15}$$

For $B = 0$, the opposite limit, equation (2) gives

$$-2E = (n + T^{1/2} + \tfrac{1}{2})^{-2}. \tag{16}$$

The half-integer radial quantum number of equation (16) for $T = m^2$ led Gay *et al* (1980) to use $T = (|m| + \frac{1}{2})^2$ to obtain 'the right low-field diamagnetic Coulomb behaviour'. In the field-free limit, this replacement produces a quasi-hydrogenic spectrum given by

$$-2E = (n + |m| + 1)^{-2} \tag{17}$$

with $|m|$ playing the role of the quantum number $l$ (of the field-free problem in spherical coordinates). By taking $T = (m + \frac{1}{2})^2$ Economou *et al* (1978) claimed to obtain the correct spectrum at the two limits above. However, as already noticed by Fonck *et al* (1980), this value does not produce the desired agreement. Regarding the work of Economou *et al*, we further add that the sign of the paramagnetic contribution in their equations (2) and (3) should be reversed.

Using equations (2) and (8) derived above we have computed and plotted figures 1 and 2. Figure 1 is akin to figure 4 of Gay *et al* (1980) and was computed assuming $T = (|m| + \frac{1}{2})^2$ as they did. For the two components, $m = \pm 3$, it shows the Landau ($E > 0$) and Coulomb ($E < 0$) regions as well as the expected $B^{-1/3}$ scaling at $E = 0$. It is easy to see that our figure 1 does not exactly agree with figure 4 of Gay *et al*. As kindly communicated to us by J-C Gay, this should be attributed to their further inclusion of the electron spin in the paramagnetic term.

Figure 2 is motivated by the experimental observations of Gay *et al* in the quasi-hydrogenic spectrum of caesium, that 'the spacing of the resonances continuously decreased from the Coulomb to the Landau regime which is almost reached for levels at $E \simeq 100\ \text{cm}^{-1}$, the spacing being $1.1\hbar\omega$ for $B = 20$ kG'. For constant $E$, according to equation (15), a plot of $n$ against $1/B$ should give a straight line. This tendency is clearly displayed in figure 2 as the energy increases.

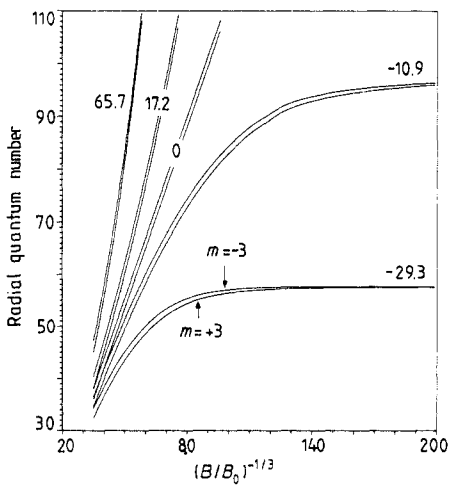


**Figure 1.** Radial quantum numbers plotted against $(B/B_0)^{-1/3}$, where $B_0 = 2.35 \times 10^9$ G, as obtained from equation (2). The numbers on each curve refers to the energy in $\text{cm}^{-1}$. The doublets correspond to $m = \pm 3$, as indicated. Note the $B^{-1/3}$ scaling at $E = 0\ \text{cm}^{-1}$ as well as the Landau ($E > 0$) and Coulomb ($E < 0$) limits.

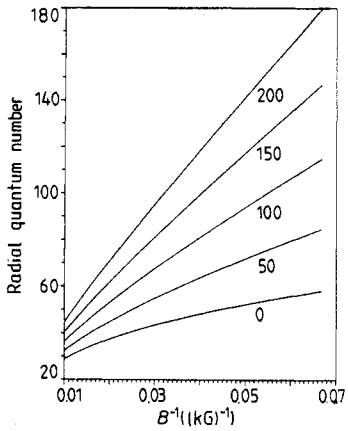


**Figure 2.** Build up of the Landau limit for $15 \leq B \leq 100$ kG. The numbers on each curve refer to the energy in $cm^{-1}$.

**Table 1.** Effect of $T = m^2$ and $T = (|m| + \frac{1}{2})^2$ on the radial quantum numbers and on the energy spacing. For fixed $m$ and $E$, the upper line corresponds to $T = (|m| + \frac{1}{2})^2$ while the lower corresponds to $T = m^2$. All quantities are calculated with $B = 20$ kG. $D$ is a measure of the relative magnitudes of $E$ and $V_c$ (see text).

| $m$ | $E$ ($cm^{-1}$) | $T$ | $n$ | $\frac{1}{\hbar\omega}\frac{dE}{dn}$ | $10^{-6}$ D |
|---|---|---|---|---|---|
| 0 | −50.0 | 0.250 | 40.667 | 2.204 47 | −32.60 |
| 0 | −50.0 | 0.0 | 41.166 | 2.204 52 | −32.60 |
| 0 | 0.0 | 0.250 | 55.797 | 1.499 97 | −17.27 |
| 0 | 0.0 | 0.0 | 56.296 | 1.500 00 | −17.27 |
| 0 | 50.0 | 0.250 | 75.534 | 1.259 72 | −6.466 |
| 0 | 50.0 | 0.0 | 76.033 | 1.259 74 | −6.466 |
| 0 | 100.0 | 0.250 | 97.751 | 1.163 81 | 2.236 |
| 0 | 100.0 | 0.0 | 98.249 | 1.163 83 | 2.236 |
| 3 | −50.0 | 12.250 | 37.009 | 2.266 25 | −33.63 |
| 3 | −50.0 | 9.000 | 37.505 | 2.266 88 | −33.63 |
| 3 | 0.0 | 12.250 | 51.832 | 1.521 02 | −17.98 |
| 3 | 0.0 | 9.000 | 52.325 | 1.521 42 | −17.98 |
| 3 | 50.0 | 12.250 | 71.392 | 1.266 90 | −7.008 |
| 3 | 50.0 | 9.000 | 71.880 | 1.267 15 | −7.006 |
| 3 | 100.0 | 12.250 | 93.523 | 1.166 83 | 1.763 |
| 3 | 100.0 | 9.000 | 94.007 | 1.167 00 | 1.767 |
| −3 | −50.0 | 12.250 | 38.371 | 2.141 21 | −31.57 |
| −3 | −50.0 | 9.000 | 38.867 | 2.141 82 | −31.57 |
| −3 | 0.0 | 12.250 | 53.834 | 1.477 39 | −16.57 |
| −3 | 0.0 | 9.000 | 54.326 | 1.477 77 | −16.57 |
| −3 | 50.0 | 12.250 | 73.775 | 1.251 14 | −5.949 |
| −3 | 50.0 | 9.000 | 74.263 | 1.251 38 | −5.946 |
| −3 | 100.0 | 12.250 | 96.102 | 1.159 64 | 2.672 |
| −3 | 100.0 | 9.000 | 96.586 | 1.159 81 | 2.677 |

To have a clear picture of the effect of the different $T$ models on the radial quantum numbers we also plotted in figures 1 and 2 the radial quantum numbers as calculated with $T = m^2$. However, over any reasonable range of parameters, any pair of such

curves perfectly overlaps. Since the values of $E$ and $B$ in figures 1 and 2 are the ones typically used in experiments, one sees that the result of using $T = m^2$ or $T = (|m| + \frac{1}{2})^2$ is essentially the same. For $B = 20$ kG the quantitative difference between the two $T$ models can be seen in table 1. From this table one sees that the spacing between resonances is much less affected than the quantum numbers (energy) themselves. Furthermore, one sees that for $E \simeq 100\ \text{cm}^{-1}$ the predicted spacing is about $1.2\hbar\omega$ in good agreement with the experimental value of $1.1\hbar\omega$ measured by Gay *et al.*

In summary, we have presented a simple analytic eigenvalue formula for the quasi-Landau spectrum. This formula is given in terms of elliptic integrals, easily generated by programmable pocket calculators, from which numerical results which are in good agreement with experiments are easily obtained. In addition, we have shown that for parameters of experimental interest $T = m^2$ or $T = (|m| + \frac{1}{2})^2$ give essentially the same result but, with the WKB approximation, $T = m^2$ should be preferred. It is also worth pointing out that equation (2) can be easily used to study hydrogenic atoms in strong magnetic fields. In particular, our equation (2) can be directly used to quantise equation (2) of the 'one-configuration' ansatz of Wunner *et al* (1981). This interesting problem will be discussed elsewhere.

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