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Two-dimensional hydrogen in a magnetic field: analytical solutions

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Abstract. Analytical solutions of the Schrödinger equation for two-dimensional hydrogen in a homogeneous magnetic field (perpendicular to the plane in which the electron is located) are found for a denumerably infinite set of field strengths. The number of solutions for the Nth excited state is N.

1. Introduction

Hydrogen in a homogeneous magnetic field is of considerable interest because of the fact that the classical system exhibits chaotic behaviour and the quantum mechanical treatment provides a rich spectrum, which can be checked experimentally (see [1, 2] and references therein). A related problem is the investigation of donor states in a magnetic field in an effective mass approximation (see e.g. [3] and references therein). It is shown here, that unlike in three dimensions, the two-dimensional Schrödinger equation can be solved analytically for a denumerably infinite set of magnetic field strengths. A possible application for this model is to donor states in a two-dimensional electron gas. The method employed is the same as that used for solving the two-electron oscillator [4] and for two electrons in a magnetic field [5]. In any of the three cases the ultimate ordinary differential equation has the form of a one-dimensional Schrödinger equation in an effective potential of the form $\alpha r^{-2} + \beta r^{-1} + \gamma r^2$, being a hybrid of a Coulomb and an oscillator potential. The first term may be interpreted as the centrifugal term. An earlier attempt [6] to solve the Schrödinger equation in the effective potential $\frac{1}{2}l(l+1)r^{-2} - Zr^{-1} + gr + \lambda r^2$ led to analytic solutions only for $g \neq 0$. Whereas the last term λr^2 can be attributed to a magnetic field in the symmetric gauge (if the two-dimensional space is considered and consequently if the centrifugal term is modified), the linear term has hardly any physical relevance. Thus, in [6] virtually the same problem was investigated, but solutions were not found for the physically relevant case $g \to 0$ (probably due to an improper ansatz).

2. Method

The Hamiltonian to be diagonalized reads†

$$H = \frac{1}{2}\left(p + \frac{1}{c}A\right)^2 - \frac{Z}{r} \tag{1}$$

† The CGS system and atomic units $\hbar = m = e = 1$ are used throughout.

where c is the velocity of light and the vector potential in the symmetric gauge is $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r}$. The magnetic field $\boldsymbol{B}$ is perpendicular to the plane in which the electron is located. In polar coordinates (r,α) within the plane and with the ansatz for the eigenfunction

$$\varphi(r) = \frac{e^{im\alpha}}{\sqrt{2\pi}} \frac{u(r)}{\sqrt{r}} \qquad m = 0, \pm 1, \pm 2, \ldots \tag{2}$$

the radial wavefunction $u(r)$ has to satisfy the radial Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}(m^2 - \frac{1}{4})\frac{1}{r^2} + \frac{1}{2}\omega_L^2 r^2 - \frac{Z}{r}\right] u(r) = [E - m\omega_L]u(r). \tag{3}$$

Here, the Larmor frequency $\omega_L = \frac{1}{2}\omega_c = B/2c$ has been introduced, E is the energy eigenvalue and m the angular momentum. Now we write $u(r)$ as a product of the asymptotic solutions (for small and large r) and a polynomial

$$u(\varrho) = e^{-\varrho^2/2} \varrho^{|m|+1/2} \sum_\nu a_\nu \varrho^\nu \tag{4}$$

where additionally the rescaled variable $\varrho = \sqrt{\omega_L} r$ has been introduced. Substitution of (4) into (3) leaves us with a recursion formula for the expansion coefficients:

$$a_0 \neq 0 \tag{5}$$

$$a_1 = -\frac{Z}{(|m| + \frac{1}{2})\sqrt{\omega_L}} a_0 \tag{6}$$

and for $\nu \geqslant 2$ we have

$$a_\nu = \frac{1}{\nu(\nu + 2|m|)} \left\{-\frac{2Z}{\sqrt{\omega_L}} a_{\nu-1} + [2(|m| + \nu - 1) - \epsilon] a_{\nu-2}\right\} \tag{7}$$

where

$$\epsilon = \frac{2E}{\omega_L} - 2m. \tag{8}$$

So far nothing has been done to guarantee normalizability of the eigenfunctions. I cannot make any necessary *and* sufficient statements on this issue. However, a *sufficient* condition for normalizability is that the series a_ν terminates at a certain $\nu = n$:

$$a_0 \neq 0, a_1 \neq 0, \ldots, a_{n-1} \neq 0, a_n = 0, a_{n+1} = 0, \ldots.$$

Due to the three-step nature of these recursion relations it is a sufficient condition for termination to ensure that two succeeding coefficents (say a_n and a_{n+1}) vanish; the rest then vanish automatically. Suppose we have calculated a_n from (5)–(7) in the form

$$a_n = F(|m|, n, \epsilon, \omega_L) a_0. \tag{9}$$

From (7) it follows that

$$a_{n+1} = \frac{1}{(n+1)(n+1+2|m|)} \left\{-\frac{2Z}{\sqrt{\omega_L}} a_n + [2(|m| + n) - \epsilon] a_{n-1}\right\}. \tag{10}$$

Now, the two conditions which guarantee $a_n = 0$ and $a_{n+1} = 0$ read

$$F(|m|, n, \epsilon, \omega_L) = 0 \tag{11}$$

and

$$\epsilon = 2(|m| + n). \tag{12}$$

These two equations are satisfied only when the energy E (or ϵ) *and* the magnetic field B (or ω_L) are considered as disposable parameters. Thus, we obtain for any n a certain number of pairs (ω_L, ϵ), for which normalizability is guaranteed. Technically, we substitute ϵ from (12) into (11) and obtain

$$F(|m|, n, 2(|m| + n), \omega_L) = 0 \tag{13}$$

which is a polynomial in $\sqrt{\omega_L}$. The zeros of (13) provide the allowed magnetic fields. The corresponding energies follow from (12) and (8):

$$E = \omega_L(n + |m| + m). \tag{14}$$

Table 1. All *allowed* Larmor frequencies ω_L and corresponding eigenvalues E for $Z = 1$, $n = 2$–10 and $m = 0$ and 1. N is the number of nodes of the radial wavefunction, indicating which excited state it is.

$m = 0$				$m = 1$			
n	ω_L^{-1}	E	N	n	ω_L^{-1}	E	N
2	0.500000E+00	0.400000E+01	1	2	0.150000E+01	0.266667E+01	1
3	0.300000E+01	0.100000E+01	2	3	0.700000E+01	0.714286E+00	2
4	0.927200E+01	0.431406E+00	3	4	0.181394E+02	0.330772E+00	3
	0.727998E+00	0.549452E+01	2		0.186059E+01	0.322478E+01	2
5	0.211168E+02	0.236778E+00	4	5	0.366510E+02	0.190991E+00	4
	0.388316E+01	0.128761E+01	3		0.834903E+01	0.838421E+00	3
6	0.403133E+02	0.148834E+00	5	6	0.642985E+02	0.124420E+00	5
	0.112570E+02	0.533000E+00	4		0.210161E+02	0.380660E+00	4
	0.929632E+00	0.645417E+01	3		0.218539E+01	0.366068E+01	3
7	0.686380E+02	0.101984E+00	6	7	0.102855E+03	0.875018E–01	6
	0.246751E+02	0.283687E+00	5		0.415559E+02	0.216576E+00	5
	0.468692E+01	0.149352E+01	4		0.958910E+01	0.938566E+00	4
8	0.107868E+03	0.741648E–01	7	8	0.154096E+03	0.648944E–01	7
	0.459214E+02	0.174211E+00	6		0.717176E+02	0.139436E+00	6
	0.130953E+02	0.610908E+00	5		0.236998E+02	0.421945E+00	5
	0.111539E+01	0.717239E+01	4		0.248615E+01	0.402228E+01	4
9	0.159781E+03	0.563272E–01	8	9	0.219800E+03	0.500456E–01	8
	0.767724E+02	0.117230E+00	7		0.113269E+03	0.971138E–01	7
	0.280095E+02	0.321320E+00	6		0.461803E+02	0.238197E+00	6
	0.543732E+01	0.165523E+01	5		0.107509E+02	0.102317E+01	5
10	0.226154E+03	0.442176E–01	9	10	0.301742E+03	0.397691E–01	9
	0.119005E+03	0.840301E–01	8		0.167984E+03	0.714353E–01	8
	0.512233E+02	0.195224E+00	7		0.787673E+02	0.152347E+00	7
	0.148274E+02	0.674429E+00	6		0.262373E+02	0.457365E+00	6
	0.129016E+01	0.775096E+01	5		0.276930E+01	0.433323E+01	5

3. Results

The simplest solutions obtained in this way read as follows: for $n = 2$ and arbitrary angular momentum m we have

$$\omega_L = \frac{Z^2}{|m| + \frac{1}{2}} \tag{15}$$

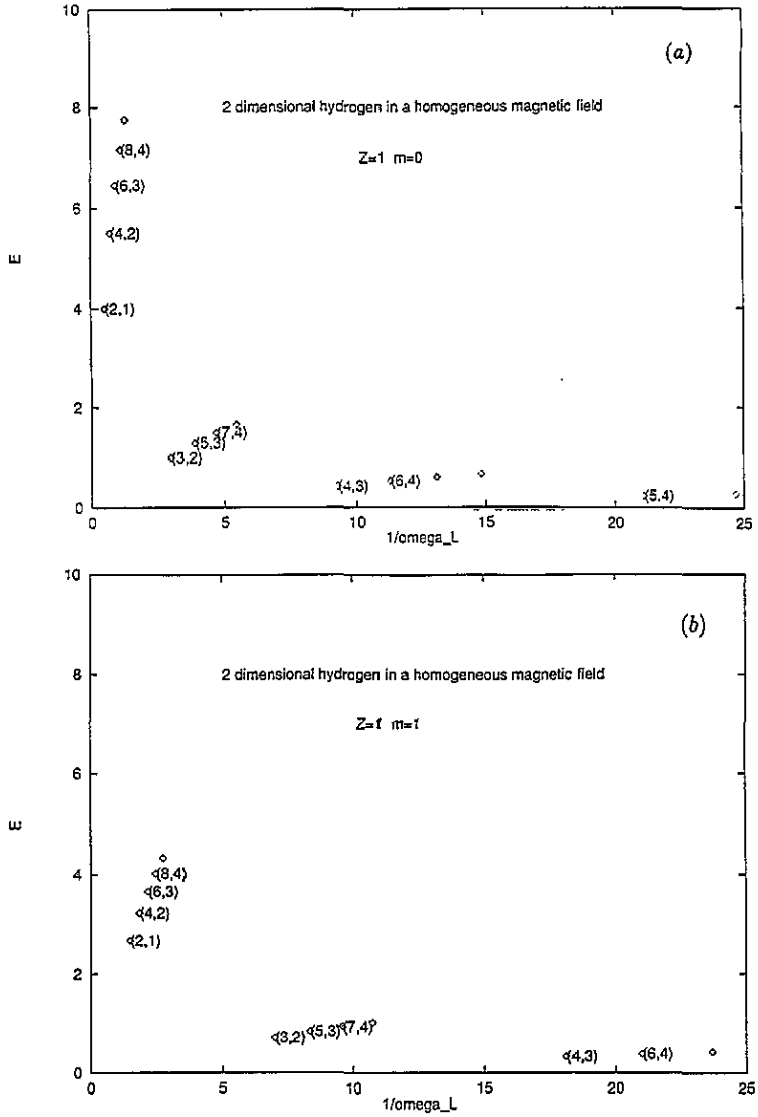

Figure 1. Eigenvalues E plotted against inverse Larmor frequencies $1/\omega_L$ for $Z = 1$ and (a) $m = 0$, (b) $m = 1$. The numbers in parentheses (n, N) are the termination index n and the number of nodes N of the corresponding radial wavefunction.

$$E = \frac{2Z^2}{(2|m|+1)}(|m| + m + 2) \tag{16}$$

$$\varphi(r) \sim \frac{e^{im\alpha}}{\sqrt{2\pi}} \exp\left(-\frac{Z^2}{(2|m|+1)} r^2\right) r^{|m|} \left[1 - \frac{Z}{(|m| + \frac{1}{2})} r\right] \tag{17}$$

and for $n = 3$ we obtain

$$\omega_L = \frac{Z^2}{4|m| + 3} \tag{18}$$

$$E = \frac{Z^2}{(4|m|+3)}(|m|+m+3) \tag{19}$$

$$\varphi(r) \sim \frac{e^{im\alpha}}{\sqrt{2\pi}} \exp\left(-\frac{Z^2}{2(4|m|+3)}r^2\right) r^{|m|}\left[1 - \frac{2Z}{2|m|+1}r + \frac{2Z^2}{(2|m|+1)(4|m|+3)}r^2\right]. \tag{20}$$

For $n \geqslant 4$ equation (13) has more than one solution. Exactly speaking, the number of solutions is $\mathrm{int}(n/2)$ (see also table 1). So far, it has not been mentioned whether the solutions found in this way are ground or excited states. It is easily seen that the wavefunction for $n = 2$ has one node (first excited state) and the solution for $n = 3$ has two nodes (second excited state). The two solutions for $n = 4$ have 2 and 3 nodes, etc. In table 1 all solutions are given for $Z = 1$, $m = 0$ and 1, and $n = 2$–10; in figure 1 some are plotted.

Two comments are in order here. Firstly, all energies obtained by this method are positive. From the solutions for $B = 0$ (which can be calculated using the conventional method familiar from three-dimensional hydrogen)

$$E_{nm}(B=0) = -\frac{Z^2}{2(n+|m|-\frac{1}{2})^2} \tag{21}$$

it is clear, that for small B all eigenvalues must be negative. Secondly, there is no ground state among our exact solutions, however, for any angular momentum we have one first excited state, two second excited states etc (see table 1). From both features we conclude that our method is particularly suited for higher excited states (Rydberg states) and high magnetic fields.

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