INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 7923–7951 PII: S0305-4470(03)63577-8

Two-dimensional hydrogen atom in a strong magnetic field

Marko Robnik and Valery G Romanovski

CAMTP—Center for Applied Mathematics and Theoretical Physics, University of Maribor, Krekova 2, SI-2000 Maribor, Slovenia

E-mail: Robnik@uni-mb.si and Valery.Romanovsky@uni-mb.si

Received 15 May 2003
Published 8 July 2003
Online at stacks.iop.org/JPhysA/36/7923

Abstract

We study the Schrödinger equation of the hydrogen atom in the (arbitrarily) strong magnetic field in two dimensions, which is an integrable and separable system. The energy spectrum is very interesting as it has infinitely many accumulation points located at the values of the Landau energy levels of a free electron in the uniform magnetic field. In the polar coordinates, the canonical (not kinetic!) angular momentum has a precise eigenvalue and we have the one-dimensional radial Schrödinger equation, which is an ordinary second-order differential equation whose analytical exact solution is unknown. We describe the qualitative properties of the energy spectrum, and we propose a semi-analytical method to numerically calculate the eigenenergies (the representation matrix of the Hamiltonian in the Landau basis is analytically calculated and is exactly known). Also, we use a number of useful analytical approximation methods, such as semiclassical approximations, the perturbation method, the variational method and the Taylor power expansion of the potential around the minimum to estimate the ground-state energy and the higher levels.

PACS numbers: 03.65.−w, 03.65.Ge, 03.65.Sq, 32.60.+i

1. Introduction

The problem of the hydrogen atom (or hydrogen-like atoms, or highly excited atoms—Rydberg atoms—also called planetary atoms; in what follows we shall simply speak of the hydrogen atom) in a strong magnetic field is an important and fascinating problem (Robnik 1981, 1982, Hasegawa *et al* 1989, Friedrich and Wintgen 1989, Ruder *et al* 1994, Blümel and Reinhardt 1997). One motivation comes from experimental physics, namely atomic spectroscopy, where we would like to understand the spectra of the highly excited hydrogen atom in the strong(est) magnetic fields available in the laboratory (up to about 10 Tesla = 10^5 G). The earliest measurements have been performed by the group of Professor Welge (Holle *et al* 1988) and

the group of Professor Kleppner (Iu *et al* 1991), although the oldest outline and suggestion for such experiments goes back to Mueller and Hughes (1974). Another phenomenon known since long ago is the quasi-Landau resonance (Garton and Tomkins 1969).

The other motivation, perhaps even older than laboratory experiments, comes from astrophysics, where hydrogen spectra in strong magnetic fields have been known since at least about 1970, e.g. in the strongly magnetic white dwarf stars (the polar magnetic field strength can be as large as up to about 5×10^8 G) whose hydrogen covered surfaces are still radiating while slowly cooling down, sometimes with additional accreted hydrogen from the interstellar space. The so-called Minkowski absorption bands, known since the 1970s, have finally been explained in terms of the so-called stationary line spectroscopy (Wunner *et al* 1985). Theoretically it has been shown (Ruder *et al* 1994 and references therein) that the energy spectrum and thus the wavelengths of the spectral lines are extremely sensitive to the strength B of the magnetic field, so they vary wildly with B. Since B in the emission region is highly nonuniform (B of a star typically is a dipole field, so it decreases inversely cubically with the distance), the line spectrum is expected to be quite blurred, easily confused with a continuous spectrum. However, the stationary spectral lines, i.e. those lines at certain $B = B_s$ where the second derivative w.r.t. B at B_s vanishes (having maximum, minimum or inflection there), step out and are easily clearly recognized. In this way, it has been possible to explain the Minkowski bands in terms of the stationary lines dominated by the emission in that B where the stationary condition is satisfied, and thus the estimate of the magnetic field strength in that emission region could be deduced. In a certain particular case (Wunner *et al* 1985) this result agrees with the determination of B through the measurement of the circular polarization of the optical continuum by Kemp *et al* (1970), and this has been quite a successful theory of atomic spectra in strong magnetic fields. Neutron stars can have polar magnetic field strengths up to 10^{13} G. There is no hydrogen, but we can have, for example, the almost completely ionized (and possibly highly excited) iron FeXXVI, in a variety of accretion scenarios, in binary systems rather than in isolated neutron stars (pulsars).

On the theoretical side, the problem of the hydrogen atom in strong (actually arbitrary) B is fascinating, because it is a *paradigm* of classical and quantal Hamiltonian nonintegrable and chaotic system (Robnik 1981, 1982, Bohigas *et al* 1986, Hasegawa *et al* 1989, Friedrich and Wintgen 1989, Stöckmann 1999), in the three-dimensional (3D) case. It is the example of quantum chaos *par excellence*. Indeed, the simple classical system described by the Lagrange function

$$\mathcal{L} = \frac{1}{2} m_e \mathbf{v}^2 + \frac{e}{c} \mathbf{A} \cdot \mathbf{v} - \frac{Qe}{r} \tag{1}$$

where $\mathbf{A}$ is the vector potential, and $\mathbf{v}$ is the velocity vector of the point charge e, moving in the magnetic field $\mathbf{B}$ and in the Coulomb electrostatic field of the central point charge Q, is generally a *nonintegrable* Hamiltonian dynamical system of the mixed type. This exhibits chaotic motion for certain initial conditions in the classical phase space and regular motion on invariant tori for other initial conditions, depending on the energy, strength of the magnetic field and on the particular initial conditions (Robnik 1981). Generally, it is predominantly regular at low energies, and chaotic at high energies. The chaos–regularity border is qualitatively defined by comparing and equating the strength of the Coulomb force with the magnetic force acting on the moving point charge e with mass m_e. Here c is the velocity of light and also $r = |\mathbf{r}|$. For clarity, in the case of an electron attracted by a Z-fold positively charged nucleus we have $e = -e_0$, and $Q = Ze_0$, where e_0 is the elementary charge and Z is the number of protons.

The Hamiltonian H as a function of coordinates $\mathbf{r}$ and the generalized *canonical* momenta $\mathbf{p}$, derived from (1) by the standard procedure, reads

$$H(\mathbf{r},\mathbf{p}) = \frac{1}{2m_e}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + \frac{Qe}{r} \tag{2}$$

describing the motion of the point charge e in the Coulomb electrostatic field and in a magnetic field

$$\mathbf{B} = \operatorname{curl}\mathbf{A}. \tag{3}$$

In particular, even if the magnetic field is just a uniform static field (time-independent) $\mathbf{B}$, for which the vector potential $\mathbf{A}$ can be written as

$$\mathbf{A} = \tfrac{1}{2}\mathbf{B}\times\mathbf{r} \tag{4}$$

we obtain H in the form

$$H(\mathbf{r},\mathbf{p}) = \frac{1}{2m_e}\mathbf{p}^2 - \frac{e}{2m_e c}\mathbf{B}\cdot\mathbf{L} + \frac{e^2}{8m_e c^2}(\mathbf{B}\times\mathbf{r})^2 + \frac{Qe}{r} \tag{5}$$

where $\mathbf{L}$ is the *canonical* angular momentum $\mathbf{L} = \mathbf{r}\times\mathbf{p}$. The Hamiltonian equations of motion are

$$\begin{aligned}\dot{\mathbf{p}} &= -\frac{\partial H}{\partial \mathbf{r}} = \frac{e}{2m_e c}\mathbf{p}\times\mathbf{B} + \frac{e^2}{4m_e c^2}\mathbf{B}\times(\mathbf{B}\times\mathbf{r}) + \frac{Qe\mathbf{r}}{r^3}\\ \dot{\mathbf{r}} &= \frac{\partial H}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m_e} - \frac{e}{2m_e c}\mathbf{B}\times\mathbf{r} = \frac{1}{m_e}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right).\end{aligned} \tag{6}$$

The total energy (2) is therefore the sum of the kinetic and of the Coulomb electrostatic potential energy, namely

$$H = \frac{1}{2}m_e\dot{\mathbf{r}}^2 + \frac{Qe}{r}. \tag{7}$$

By substitution in equations (6) we can easily arrive at Newton's equations of motion

$$m_e\ddot{\mathbf{r}} = m_e\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2} = \frac{e}{m_e c}(m_e\dot{\mathbf{r}})\times\mathbf{B} + \frac{Qe\mathbf{r}}{r^3} \tag{8}$$

thereby eliminating the canonical momenta and writing them in terms of the kinetic momentum $\mathbf{P} = m_e\dot{\mathbf{r}}$. Clearly, if there is no Coulomb field (i.e. if $Q = 0$ in the last term in equation (7)) then the vector $\mathbf{P} = m_e\dot{\mathbf{r}}$ has a constant length $P = |\mathbf{P}| = \text{const}$, and simply precesses around the vector $\mathbf{B}$ with the angular cyclotron frequency $\omega = |eB|/(m_e c)$ (twice the Larmor frequency), in the mathematically positive sense around the z-axis if $eB < 0$ and negative if $eB > 0$. Thus we have an integrable system. However, the Coulomb interaction destroys the separability and the integrability of the system as was shown first in Robnik (1981), in the 3D case.

It is easy to show that $\mathbf{L}$ is not conserved, whilst $L_z = \mathbf{B}\cdot\mathbf{L}/B$ is a conserved quantity, the z-component of the angular momentum, chosen as parallel to the vector $\mathbf{B}$. Namely, it follows from equation (6) that

$$\dot{\mathbf{L}} = \frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = -\frac{e}{2m_e c}\mathbf{B}\times\mathbf{L} + \frac{e^2}{4m_e c^2}(\mathbf{B}\cdot\mathbf{r})(\mathbf{r}\times\mathbf{B}) \tag{9}$$

and consequently

$$B\dot{L}_z = B\frac{\mathrm{d}L_z}{\mathrm{d}t} = \mathbf{B}\cdot\dot{\mathbf{L}} = 0 \tag{10}$$

so that indeed L_z is a constant of motion, whilst $\mathbf{L}$ is not! Of course, conservation (invariance) of L_z along with the total energy H is not enough to preserve the integrability of the system.

One (scalar) integral of motion is missing for that, and in fact there is no such integral, implying the nonintegrability and chaoticity of the 3D system, as has been shown originally in Robnik (1981). For sufficiently small B, the second term, quadratic in B, in equation (9) can be neglected and then we have approximately just a precession of $\mathbf{L}$ around the vector $\mathbf{B}$ at the Larmor frequency ($\omega_L = \omega/2$) and therefore approximate integrability (KAM regime, with invariant tori almost everywhere).

Even if the 3D problem is chaotic and therefore analytically not solvable, the two-dimensional (2D) case, which is an integrable and even separable system, is still very interesting, from the point of view of mathematical physics, although still not analytically exactly solvable, and it sheds some light on the aspects of the 3D problem. In this paper we deal with the 2D problem only.

Let us now specialize to the 2D case $z = 0$ by rewriting the Lagrange function (1) in polar coordinates (ρ, ϕ)

$$\mathcal{L} = \frac{m_e}{2}(\dot{\rho}^2 + \rho^2\dot{\varphi}^2) + \frac{eB}{2c}\rho^2\dot{\varphi} - \frac{Qe}{\rho}. \tag{11}$$

After introducing the standard notations for canonical momenta

$$p_\rho = \frac{\partial \mathcal{L}}{\partial \dot{\rho}} = m_e\dot{\rho} \qquad p_\varphi = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} = m_e\rho^2\dot{\varphi} + \frac{eB}{2c}\rho^2 \tag{12}$$

and performing the standard procedure to construct the Hamiltonian function $\mathcal{H}$ of the system (11)

$$\mathcal{H} = p_\rho\dot{\rho} + p_\varphi\dot{\varphi} - \mathcal{L} \tag{13}$$

we obtain

$$\mathcal{H} = \frac{p_\rho^2}{2m_e} + \frac{p_\varphi^2}{2m_e\rho^2} - \frac{eBp_\varphi}{2m_ec} + \frac{e^2B^2\rho^2}{8m_ec^2} + \frac{Qe}{\rho}. \tag{14}$$

Here φ is a cyclic variable, so again we see immediately that p_φ is a constant of motion, because

$$\dot{p}_\varphi = -\frac{\partial \mathcal{H}}{\partial \varphi} = 0 \tag{15}$$

and therefore

$$\dot{\varphi} = \frac{\partial \mathcal{H}}{\partial p_\varphi} = \frac{p_\varphi}{m_e\rho^2} - \frac{eB}{2m_ec} \tag{16}$$

and consequently

$$\varphi(t) = \int_{t_0}^{t}\left(\frac{p_\varphi}{m_e\rho^2} - \frac{eB}{2m_ec}\right)\mathrm{d}t + \varphi(t_0) \tag{17}$$

can be immediately integrated once $\rho(t)$ as a function of time t is known. The latter is of course obtained as a solution of the ordinary second-order differential equation for ρ, which follows from the Hamilton equations generated by $\mathcal{H}$ in equation (14), namely

$$m_e\ddot{\rho} = -\frac{\partial \mathcal{H}}{\partial \rho} = \frac{p_\varphi^2}{m_e\rho^3} - \frac{e^2B^2}{4m_ec^2}\rho + \frac{Qe}{\rho^2}. \tag{18}$$

If we choose a coordinate system rotating at Larmor rotation frequency $\omega_L = \omega/2$ (one half cyclotron frequency!), we can eliminate in equation (11) and thus in equation (14) the paramagnetic term (linear in B), which is also clear in equation (17), getting the most simple (2D) form of the Hamiltonian as was proposed and studied in Robnik (1981), namely

$$\mathcal{H} = \frac{p_\rho^2}{2m_e} + \frac{p_\varphi^2}{2m_e\rho^2} + \frac{e^2B^2\rho^2}{8m_ec^2} + \frac{Qe}{\rho}. \tag{19}$$

The *canonical angular momentum* **L** is different from the *kinetic angular momentum* **l**, namely we have the definition

$$\mathbf{l} = \mathbf{r} \times m_e \mathbf{v} \tag{20}$$

and thus (from the second equation of (6))

$$\mathbf{l} = \mathbf{L} - \frac{e}{2c}\mathbf{r} \times (\mathbf{B} \times \mathbf{r}). \tag{21}$$

The z-component (parallel to **B**) is equal to

$$l_z = L_z - \frac{eB}{2c}\rho^2. \tag{22}$$

When going over to the quantum mechanics of our problem, we apply the canonical quantization rule in the ordinary coordinate space, thus replacing momentum **p** by the operator

$$\hat{\mathbf{p}} = -\mathrm{i}\hbar\frac{\partial}{\partial \mathbf{r}}. \tag{23}$$

As can be verified quantum mechanically, for the angular momenta, we have precisely equation (21)

$$\hat{\mathbf{l}} = \hat{\mathbf{L}} - \frac{e}{2c}\mathbf{r} \times (\mathbf{B} \times \mathbf{r}) \tag{24}$$

and for the z-component

$$\hat{l}_z = \hat{L}_z - \frac{eB}{2c}\rho^2. \tag{25}$$

Therefore, for the expectation values we have

$$\langle \hat{l}_z \rangle = L_z - \frac{eB}{2c}\langle \rho^2 \rangle \tag{26}$$

where $\hat{L}_z$ in polar coordinates with the polar angle φ is equal to

$$\hat{L}_z = -\mathrm{i}\hbar\frac{\partial}{\partial \varphi} = \hat{p}_\varphi \tag{27}$$

and is a conserved quantity, with the eigenvalue L_z, which commutes with the Hamilton operator

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_e} - \frac{eB}{2m_e c}\hat{L}_z + \frac{e^2B^2}{8m_e c^2}\rho^2 + \frac{Qe}{\rho}. \tag{28}$$

Using equation (23) and the polar coordinates (ρ, φ) we obtain the Schrödinger equation

$$\hat{H}\psi = E\psi \tag{29}$$

which is fully written as

$$-\frac{\hbar^2}{2m_e}\left\{\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial \psi}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 \psi}{\partial \varphi^2}\right\} + \mathrm{i}\hbar\frac{eB}{2m_e c}\frac{\partial \psi}{\partial \varphi} + \frac{e^2B^2}{8m_e c^2}\rho^2\psi + \frac{Qe}{\rho}\psi = E\psi. \tag{30}$$

A shorter version of this paper has been published in Robnik and Romanovski (2002).

2. Preliminaries of the quantum mechanical problem

Let us briefly examine the quantum mechanical problem by considering first the free point charge (of mass m_e and charge e) in a homogeneous constant magnetic field $\mathbf{B}$, which is a well-known problem (Landau and Lifshitz 1997).

We start from equation (2) by ignoring the Coulomb term and choosing an appropriate gauge for $\mathbf{A}$.

Since $\hat{\mathbf{p}} = -\mathrm{i}\hbar\partial/\partial\mathbf{r}$ we see

$$\hat{\mathbf{p}}\mathbf{A} - \mathbf{A}\hat{\mathbf{p}} = -\mathrm{i}\hbar \operatorname{div}\mathbf{A} \tag{31}$$

and thus if we choose the Coulomb gauge $\operatorname{div}\mathbf{A} = 0$, the commutator in equation (31) vanishes, and then the Schrödinger energy operator becomes

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_e} - \frac{e}{m_e c}\mathbf{A}\cdot\hat{\mathbf{p}} + \frac{e^2}{2m_e c^2}\mathbf{A}^2. \tag{32}$$

We shall work in polar coordinates (ρ, φ) (i.e. polar coordinates in the (x, y)-plane) by choosing the vector potential

$$\mathbf{A}_P = (A_\rho, A_\varphi) = \left(0, \tfrac{1}{2}B\rho\right) \tag{33}$$

whose Cartesian coordinates are

$$\mathbf{A}_P = (A_x, A_y) = \left(-\tfrac{1}{2}By, \tfrac{1}{2}Bx\right). \tag{34}$$

We make the separation

$$\psi = \psi(x, y) = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{\mathrm{i}m\varphi}R_m(\rho) \tag{35}$$

and inserting it into equation $\hat{H}\psi = E\psi$, namely equation (30), we find

$$-\frac{\hbar^2}{2m_e}\left[R'' + \frac{1}{\rho}R' - \frac{m^2}{\rho^2}R\right] - \frac{m\hbar\omega}{2}\operatorname{sign}(eB)R + \frac{m_e\omega^2}{8}\rho^2 R = E_{m,n_\rho}R \tag{36}$$

where m is the *canonical angular momentum quantum number*, $m = 0, \pm1, \pm2, \pm3, \ldots$, so that (see equation (27)) the eigenvalue of $\hat{L}_z$ is $L_z = m\hbar$, whilst n_ρ will be the radial quantum number counting the number of nodes of the radial wavefunction $R_{m,n_\rho}(\rho)$, so $n_\rho = 0, 1, 2, 3, \ldots$. The total energy now is

$$E = E_{m,n_\rho}. \tag{37}$$

The radial Schrödinger equation for R_{m,n_ρ} in the form (36) can be solved elementary with the result (Landau and Lifshitz 1997)

$$R_{m,n_\rho}(\rho) = C_{|m|,n_\rho}\,\mathrm{e}^{-\xi/2}\xi^{|m|/2}w_{|m|,n_\rho}(\xi) \tag{38}$$

where

$$w_{|m|,n_\rho}(\xi) = F\left(-n_\rho, \tfrac{1}{2}(|m|+1), \xi\right) \tag{39}$$

is the confluent hypergeometric series ($F = {}_1F_1$) and

$$\xi = \frac{|eB|}{2c\hbar}\rho^2 \tag{40}$$

is the dimensionless variable proportional to ρ^2. R_{m,n_ρ} depends only on $|m|$, the sign of m does not affect its value. Therefore we have now

$$E_{m,n_\rho} = \hbar\omega\left(n_\rho + \frac{|m| - \operatorname{sign}(eB)m}{2} + \frac{1}{2}\right) \tag{41}$$

and by introducing the notation

$$n = n_\rho + \frac{|m| - \mathrm{sign}(eB)m}{2} \tag{42}$$

for the main quantum number n we write the energy spectrum as

$$E_{m,n_\rho} = \hbar\omega\left(n + \tfrac{1}{2}\right) \tag{43}$$

which is *infinitely degenerate*, but *discretely*, because for a given $n \geqslant 0$ there are infinitely many possibilities for n_ρ and m satisfying equation (42), namely

$$n_\rho = n + \frac{\mathrm{sign}(eB)m - |m|}{2} \tag{44}$$

where, in the case that $\mathrm{sign}(eB)$ is positive, m can have any non-negative integer value, or any negative integer value m whose $|m| \leqslant n$. This equation (43) is the Landau energy spectrum of a free point charge e in a constant homogeneous magnetic field B (Landau and Lifshitz 1997, p 455).

The general solution at the energy (41) of the Schrödinger equation in the (x, y)-plane can now be written

$$\psi_n(x, y) = \psi_n(\rho, \varphi) = \frac{1}{\sqrt{2\pi}} \sum_{m,n_\rho} b_{m,n_\rho}\, \mathrm{e}^{\mathrm{i}m\varphi} R_{m,n_\rho}(\rho) \tag{45}$$

where b_{m,n_ρ} are the expansion coefficients and summation runs over all m and n_ρ compatible with the fixed value of n as given in equation (42). The infinite discrete degeneracy of the energy spectrum is due to the continuous translational invariance of the underlying Hamilton system in the plane perpendicular to the magnetic field vector.

Next we would like to investigate the physical meaning of the quantum number m which, when multiplied by $\hbar$, is the eigenvalue of the canonical angular momentum L_z. First we calculate the expectation value of ρ^2. A straightforward calculation of the expectation value of ρ^2 yields (see also equation (89))

$$\langle\rho^2\rangle = \frac{2\hbar c}{|eB|}(2n_\rho + |m| + 1). \tag{46}$$

So the physical interpretation is as follows. n_ρ is the number of radial nodes of $R(\rho)$ and measures the degree of excitation, whilst m measures the distance of the electron from the origin. If $\langle\rho^2\rangle$ increases we might think semiclassically in terms of the cyclotron motion, either the centre of the cyclotron motion is close to the origin and the average radius of the cyclotron motion is very large, meaning high energies if $\mathrm{sign}(eB)m$ is negative, or the centre of the cyclotron motion is very far away from the origin while the radius of the cyclotron orbit is small, much smaller than the distance from the origin to the centre. In short, large $|m|$ means that the electron is far away from the origin, and if there is a Coulomb centre of attraction at the origin, it would act like a small perturbation to the cyclotron Landau energy levels. It would lift the infinite degeneracy of the Landau energy spectrum but obviously in such a way that those eigenstates located far away from the Coulomb centre (perturber) would be very close to the corresponding Landau level, implying that the spectrum has accumulation points, in fact infinitely many, located at precisely the Landau levels (see equations (41) and (43)) of the free electron in a magnetic field B. The energy spectrum is schematically shown in figure 1.

The expectation value of the kinetic angular momentum is according to equation (26), using equation (46), equal to

$$\langle l_z\rangle = L_z - \frac{eB}{2c}\langle\rho^2\rangle = m\hbar - \mathrm{sign}(eB)(|m| + 1 + 2n_\rho)\hbar \tag{47}$$

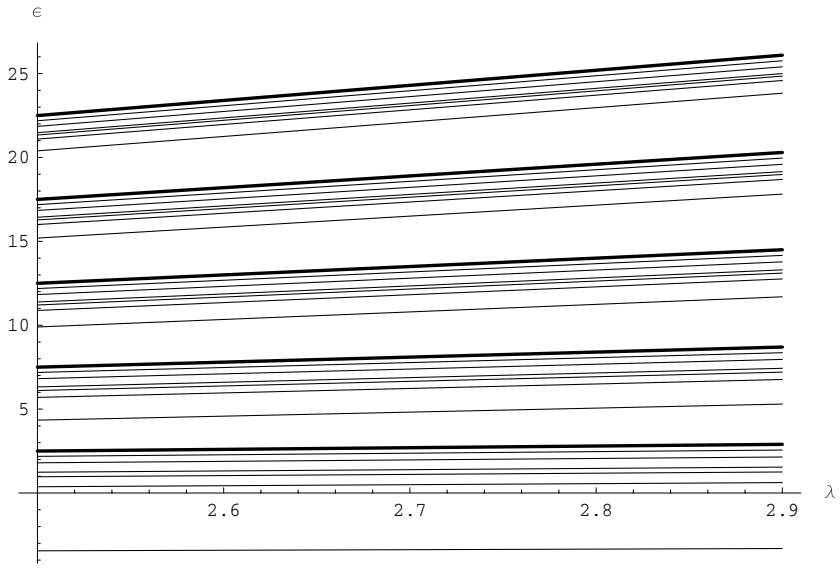

Figure 1. The first five ($n = 0, 1, 2, 3, 4$) energy levels $\tilde{\epsilon}$ for $m = 0, -1, -2, -3, -10, -50$, for the range of $\lambda \in [2.5, 2.9]$; they accumulate to the 'fat' line $(2n + 1)\lambda$.

and thus

$$\begin{aligned}\langle l_z\rangle &= -\hbar\,\mathrm{sign}(eB)(-\mathrm{sign}(eB)m + |m| + 1 + 2n_\rho)\\ &= -2\hbar\,\mathrm{sign}(eB)\left(n + \tfrac{1}{2}\right) = -2\,\mathrm{sign}(eB)E_n/\omega \end{aligned} \tag{48}$$

so that $\langle l_z\rangle$ is always positive if $eB < 0$ (e.g. electron in positively oriented $B > 0$), and negative if $eB > 0$. This is exactly what we expect intuitively based on the classical and semiclassical picture. Also, the minimum absolute value of the average kinetic angular momentum is precisely $\hbar$ (when the main Landau quantum number is equal to zero, $n = 0$, i.e. for the lowest Landau state). From equation (48) we see that the energy eigenvalue uniquely determines the absolute value of the average kinetic angular momentum, and the sign is determined by the sign of eB.

The 3D hydrogen atom in the magnetic field is a nonintegrable and chaotic system (Robnik 1981), whilst the 2D one is separable (in polar coordinates) and therefore integrable. We now go back to the Hamilton operator (28) and set up the corresponding Schrödinger equation for the 2D problem, for the separated wavefunction $\psi(\rho)\exp(\mathrm{i}m\varphi)$ in polar coordinates (ρ, φ), where we use the fact that $\hat{L}_z\psi = -\mathrm{i}\hbar\frac{\partial}{\partial\varphi}\psi = m\hbar\psi$. Thus, we obtain for the radial wavefunction ψ

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \left[\frac{2m_eE}{\hbar^2} - \frac{2m_eQe}{\hbar^2\rho} - \left(\frac{m}{\rho} - \frac{eB}{2\hbar c}\rho\right)^2\right]\psi = 0. \tag{49}$$

Let us now introduce natural units in such a way that we shall obtain the Schrödinger equation in a nice dimensionless form. We shall now specify the point charges as $e = -e_0$ and $Q = Ze_0$. The length is measured in units of Bohr radius a_B

$$\rho = a_B x \qquad a_B = \frac{\hbar^2}{m_e e_0^2}. \tag{50}$$

Another quantity with the dimension of length is the Landau radius b

$$b = \sqrt{\frac{\hbar c}{e_0|B|}} \tag{51}$$

and the unit of energy will be one Rydberg, equal to $e_0^2/(2a_B)$, so that the dimensionless energy is

$$\tilde{\epsilon} = \frac{2a_B E}{e_0^2} \tag{52}$$

and finally the unit of magnetic field strength will be such that

$$\lambda = \left(\frac{a_B}{b}\right)^2 = B/B_0 \qquad B_0 = \frac{m_e^2 e_0^3 c}{\hbar^3} \tag{53}$$

and for e_0 and m_e being the elementary charge and the electron's mass we obtain

$$B_0 = \frac{m_e^2 e_0^3 c}{\hbar^3} = 2.3506 \times 10^9 \text{ Gauss} = 2.3506 \times 10^5 \text{ Tesla} \tag{54}$$

so indeed a very strong magnetic field not available in a laboratory, but in the astrophysical context mentioned in the introduction. So λ is a linear measure of the strength of the magnetic field, such that $\lambda = 1$ means $B = B_0$. With these conventions we find the dimensionless fundamental equation

$$\psi'' + \frac{1}{x}\psi' + \left[\tilde{\epsilon} + m\lambda \,\mathrm{sign}(eB) + \frac{2Z}{x} - \frac{m^2}{x^2} - \frac{\lambda^2}{4}x^2\right]\psi = 0 \tag{55}$$

and after introducing the *reduced energy* ϵ

$$\epsilon = \tilde{\epsilon} + m\lambda \,\mathrm{sign}(eB) \tag{56}$$

we have

$$\psi'' + \frac{1}{x}\psi' + \left[\epsilon + \frac{2Z}{x} - \frac{m^2}{x^2} - \frac{\lambda^2}{4}x^2\right]\psi = 0. \tag{57}$$

This is the fundamental radial ordinary second-order differential equation for the radial wavefunction ψ as a function of the dimensionless polar radius x, that we are going to study.

3. The representation of the Hamilton operator in the Landau basis

From now on the quantum number m (canonical angular momentum number) will be considered fixed unless stated otherwise explicitly. We are going to find a solution of our problem (57) by finding the eigenvalues of the Hamilton operator

$$\begin{aligned}\hat{H}(\psi) &\equiv -\psi''(x) - \frac{\psi'(x)}{x} + \left(\frac{m^2}{x^2} - \frac{2Z}{x} + \frac{x^2\lambda^2}{4}\right)\psi(x) \\ &= \tilde{H}(\psi) - \frac{2Z}{x}\psi(x)\end{aligned} \tag{58}$$

where

$$\tilde{H}(\psi) \equiv -\psi''(x) - \frac{\psi'(x)}{x} + \left(\frac{m^2}{x^2} + \frac{x^2\lambda^2}{4}\right)\psi(x). \tag{59}$$

Then

$$H_{ks} = 2\pi \int_0^\infty x\psi_k(x)\hat{H}(\psi_s)\,\mathrm{d}x = \epsilon_s\delta_{ks} - 4\pi Z\int_0^\infty \psi_k(x)\psi_s(x)\,\mathrm{d}x. \tag{60}$$

Here ϵ_s are the eigenvalues of the operator $\tilde{H}$, and in fact they are exactly the Landau levels (41), now in dimensionless form, where $s = n_\rho = 0, 1, 2, \ldots$,

$$\epsilon_s = \lambda(2s + 1 + |m|) \tag{61}$$

such that the full energy $\tilde{\epsilon}$ is equal to

$$\tilde{\epsilon}_s = \epsilon_s - m\lambda \,\mathrm{sign}(eB) = \lambda(2s + 1 + |m| + m) \tag{62}$$

because we chose $\mathrm{sign}(eB) = -1$, as $e = -e_0$ and $B > 0$. Here $\psi_s(x)$ is the sth (Landau) eigenfunction of $\tilde{H}$, where s is exactly the number of its nodes. Therefore, to complete our task we have to diagonalize the operator $\hat{H}$, i.e. its matrix H_{ks}. There are three steps: first, to show that the Landau basis of the eigenfunctions of the operator $\tilde{H}$ is complete (in Hilbert space of all ψ radial functions) (which is demonstrated below); secondly, to calculate the matrix elements H_{ks} (which is done exactly and analytically below); and thirdly, to diagonalize the H_{ks} matrix (which cannot be done exactly analytically, but only numerically). It is important to stress that the functional dependence of H_{ks} on λ, and of course on Z, will be exactly known, namely the integral in the second term of equation (60) is exactly proportional to $\sqrt{\lambda}$, as will be shown below. This is very important, because it means that the matrix H_{ks} has to be calculated (analytically and exactly) only once (see equations (82) and (86)) and consequently the energy spectrum can be obtained at any λ and Z by a diagonalization of equation (60). This is one of the major merits of this paper.

We proceed by constructing the orthonormal Landau eigenbasis $\psi_s(x)$, i.e. the normalized solutions of

$$\tilde{H}(\psi_s) \equiv -\psi_s''(x) - \frac{\psi_s'(x)}{x} + \left(\frac{m^2}{x^2} + \frac{x^2\lambda^2}{4}\right)\psi_s(x) = \epsilon_s\psi_s. \tag{63}$$

The substitution

$$y = \frac{\lambda}{2}x^2 \tag{64}$$

in equation (63) yields

$$\left(-\frac{m^2}{4y} - \frac{y}{4} + \frac{\epsilon}{2\lambda}\right)\psi(y) + \psi'(y) + y\psi''(y) = 0. \tag{65}$$

This equation has a solution

$$\mathrm{e}^{-\frac{y}{2}} y^{\frac{|m|}{2}} {}_1F_1\left(\frac{-\epsilon + \lambda + |m|\lambda}{2\lambda}, 1 + |m|, y\right) \tag{66}$$

with $F(a, b, z) \stackrel{\mathrm{def}}{=} {}_1F_1\left[\begin{smallmatrix} a \\ b \end{smallmatrix}; z\right]$ being the confluent hypergeometric function which becomes a polynomial if

$$\frac{-\epsilon + \lambda + |m|\lambda}{2\lambda} = -s \tag{67}$$

where $s = n_\rho$ is a non-negative integer equal to the number of nodes n_ρ of the radial eigenfunction.

Therefore, the spectrum of the equation (63) is precisely (61), where $s = 0, 1, 2, \ldots$ and the corresponding wavefunctions are

$$\psi_s(x) = a_s \,\mathrm{e}^{-\frac{\lambda}{4}x^2} x^{|m|} {}_1F_1\left(-s, 1 + |m|, \frac{\lambda}{2}x^2\right). \tag{68}$$

Using the interrelation between the confluent hypergeometric function and the generalized Laguerre polynomials $L_n^{|m|}(z)$,

$$L_n^{|m|}(z) = \frac{(n + |m|)!}{n!|m|!} F(-n, |m| + 1, z) \tag{69}$$

we can write the formula (68) in the form

$$\psi_s(x) = a_s \frac{|m|!s!}{(|m|+s)!}\, \mathrm{e}^{-\frac{\lambda}{4}x^2} x^{|m|} L_s^{|m|}\left(\frac{\lambda}{2}x^2\right). \tag{70}$$

Now from the normalizing condition

$$2\pi \int_0^\infty x\psi_s^2(x)\,\mathrm{d}x = 1 \tag{71}$$

and the orthogonality relation for Laguerre polynomials

$$\int_0^{+\infty} \mathrm{e}^{-u} u^{|m|} L_n^{|m|}(u) L_k^{|m|}(u)\,\mathrm{d}u = \begin{cases} 0 & \text{if} \quad n \neq k \\ \Gamma(|m|+1)\binom{n+|m|}{n} & \text{if} \quad n = k \end{cases} \tag{72}$$

we have that

$$a_s = \sqrt{\frac{\lambda^{|m|+1}(|m|+s)!^2}{2^{|m|+1}\pi\binom{|m|+s}{s}|m|!^2 s!^2 \Gamma(1+|m|)}}. \tag{73}$$

Therefore

$$\psi_s(x) = b_s\, \mathrm{e}^{-\frac{\lambda}{4}x^2} x^{|m|} L_s^{|m|}\left(\frac{\lambda}{2}x^2\right) \tag{74}$$

where

$$b_s = \sqrt{\frac{\lambda^{|m|+1}}{2^{|m|+1}\pi\binom{|m|+s}{s}|m|!}}. \tag{75}$$

Now let us show that the orthonormal system $\psi_s(x)$, $s = 0, 1, \ldots$ is a complete basis of the Hilbert space $L^2(0, +\infty)$. To this end it is sufficient to prove that the set

$$\left\{\mathrm{e}^{-\frac{\lambda}{4}x^2} x^\alpha x^{2n}\right\}_{n=0}^\infty \tag{76}$$

is dense in $L^2(0, +\infty)$. Here α is a real number $\alpha > -1/2$. Indeed, an arbitrary function $h(x)$ from $L^2(0, +\infty)$ we can write in the form

$$h(x) = \mathrm{e}^{-\frac{\lambda}{4}x^2} x^\alpha f(\sqrt{\lambda}x). \tag{77}$$

We need to show that for any $\epsilon > 0$ there exists a polynomial $t(x^2)$ such that

$$I(h) \equiv \int_0^{+\infty} \left(\mathrm{e}^{-\frac{\lambda}{4}x^2} x^\alpha [f(\sqrt{\lambda}x) - t(x^2)]\right)^2 \mathrm{d}x < \epsilon. \tag{78}$$

After the substitution $y = \lambda x^2$ we obtain

$$\begin{aligned} I(h) &= \text{const} \int_0^{+\infty} (\mathrm{e}^{-y/2} y^{\alpha/2-1/4} [f(\sqrt{y}) - t(y/\lambda)])^2\,\mathrm{d}y \\ &= \text{const} \int_0^{+\infty} (\mathrm{e}^{-y} y^\beta [f(\sqrt{y}) - \tilde{t}(y)])^2\,\mathrm{d}y < \epsilon, \end{aligned} \tag{79}$$

where $\beta = (2\alpha - 1)/2$ and $\tilde{t}(y) = t(y/\lambda)$. Note that $h(x) \in L^2(0, +\infty)$ yields that $\mathrm{e}^{-y/2} y^{\alpha/2-1/4} f(\sqrt{y}) \in L^2(0, +\infty)$. Therefore, according to (Szegö 1959, ch. 5.7), there is a polynomial $\tilde{t}(y)$ satisfying equation (79). This completes the proof of the completeness of the Landau basis at any λ.

Now we calculate the matrix elements (60). We can check that

$$L_k^{|m|}\left(\frac{\lambda}{2}x^2\right) L_s^{|m|}\left(\frac{\lambda}{2}x^2\right) = \sum_{u=0}^{k+s} \left(\sum_{j=0}^{u} \frac{(-1)^u \binom{k+|m|}{k-j}\binom{s+|m|}{s-u+j}}{j!\,(u-j)!}\right) \left(\frac{\lambda}{2}\right)^u x^{2u}. \tag{80}$$

Note that

$$\int_0^{+\infty} x^{2|m|+2u+v}\,\mathrm{e}^{-\frac{\lambda}{2}x^2}\,\mathrm{d}x = 2^{-\frac{1}{2}+|m|+u+\frac{v}{2}}\lambda^{-\frac{1}{2}-|m|-u-\frac{v}{2}}\Gamma\left(\frac{1}{2}+|m|+u+\frac{v}{2}\right). \tag{81}$$

Then, using equations (80) and (81) with $v = 0$ we obtain

$$\begin{aligned} A_{ks} = \int_0^{\infty} \psi_k(x)\psi_s(x)\,\mathrm{d}x &= b_k b_s \sum_{u=0}^{k+s}\left(\sum_{j=0}^{u}\frac{(-1)^u\binom{k+|m|}{k-j}\binom{s+|m|}{s-u+j}}{j!\,(u-j)!}\right) \\ &\quad\times\left(\frac{\lambda}{2}\right)^u 2^{-\frac{1}{2}+|m|+u}\lambda^{-\frac{1}{2}-|m|-u}\Gamma\left(\frac{1}{2}+|m|+u\right) \\ &= \frac{\lambda^{1/2}\sqrt{k!s!(k+|m|)!(s+|m|)!}}{2^{|m|+1}\sqrt{2\pi}}\sum_{u=0}^{k+s}\frac{(-1)^u(2|m|+2u-1)!!}{2^u} \\ &\quad\times\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!} \end{aligned} \tag{82}$$

To simplify the obtained expression we rewrite the sum in the form

$$\begin{aligned} &\sum_{u=0}^{s+k}\frac{(-1)^u(2|m|+2u-1)!!}{2^u}\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!} \\ &\qquad = S_1 + S_2 \end{aligned}$$

where

$$\begin{aligned} S_1 &= \sum_{u=0}^{s}\frac{(-1)^u(2|m|+2u-1)!!}{2^u} \\ &\quad\times\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!} \end{aligned}$$

and

$$\begin{aligned} S_2 &= \sum_{u=s+1}^{k+s}\frac{(-1)^u(2|m|+2u-1)!!}{2^u} \\ &\quad\times\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!} \\ &= \sum_{h=0}^{k-1}\frac{(-1)^{h+s+1}(2|m|+2h+2s+1)!!}{2^{h+s+1}} \\ &\quad\times\sum_{v=0}^{s}\frac{1}{(|m|+v+h+1)!(k-v-h-1)!(|m|+s-v)!v!(v+h+1)!(s-v)!}, \end{aligned}$$

where, to obtain this expression for S_2, we can set $u = h+s+1$, $j = v+h+1$. Note that, in fact, it is sufficient to consider only j between $h+1$ and $h+s+1$, because $\frac{1}{(-h-1+j)!} = 0$ if $j < h+1$.

To sum the inner sum in S_1 we write it as

$$\sum_{j=0}^{\infty} t_j$$

where

$$t_j = \frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!}$$

and here we are in the position to replace the finite sum by the infinite sum because again $\frac{1}{(u-j)!} = 0$ if $j > u$.

Computing we obtain

$$\frac{t_{j+1}}{t_j} = -\frac{(j-k)(j-|m|-u)(j-u)}{(j+|m|+1)(j+s-u+1)(j+1)}$$

Hence, using the algorithm from Petkovšek *et al* (1996, p 36) (which, actually, follows from the definition of hypergeometric functions), we conclude that

$$\sum_{j=0}^{u} t_j = \sum_{j=0}^{\infty} t_j = \frac{1}{|m|!k!(|m|+u)!(s-u)!u!}\,{}_3F_2\left[\begin{matrix} -k & -|m|-u & -u \\ |m|+1 & s-u+1 & \end{matrix}; -1\right]$$

and, therefore,

$$S_1 = \sum_{u=0}^{s} \frac{(-1)^u(2|m|+2u-1)!!}{2^u|m|!k!(|m|+u)!(s-u)!u!}\,{}_3F_2\left[\begin{matrix} -k & -|m|-u & -u \\ |m|+1 & s-u+1 & \end{matrix}; -1\right] \tag{83}$$

Similarly,

$$S_2 = \sum_{h=0}^{k-1} \frac{(-1)^{h+s+1}(2|m|+2h+2s+1)!!}{2^{h+s+1}(|m|+h+1)!(k-h-1)!(|m|+s)!(h+1)!s!} \times {}_3F_2\left[\begin{matrix} h+1-k & -|m|-s & -s \\ h+2|m|+h+2 & & \end{matrix}; -1\right]. \tag{84}$$

Therefore, finally we obtain

$$H_{ks} = \epsilon_s\delta_{ks} - 4\pi Z A_{ks}, \tag{85}$$

where

$$A_{ks} = \frac{\lambda^{1/2}\sqrt{k!s!(k+|m|)!(s+|m|)!}}{2^{|m|+1}\sqrt{2\pi}}\,(S_1+S_2) \tag{86}$$

with S_1 and S_2 defined by equations (83) and (84), respectively.

Note that we had to split the sum in equation (82) into two parts, S_1 and S_2, because otherwise using the algorithm of Petkovšek *et al* (1996) we would encounter during the calculations the indeterminicity $0 \cdot \infty$.

This completes our calculation of the matrix H_{ks} representing $\hat{H}$ from equation (58) in the λ-Landau basis, as given in equations (85)–(86). Note that the matrix is analytically exactly known and computable, and the dependence on λ and Z explicitly known, so that the matrix must be in fact calculated only once (this is quite an intensive procedure regarding CPU time), and then the diagonalization of H_{ks} can be performed for any λ and Z.

To compute the diagonal elements A_{kk} it is more convenient to use the formula (A.3) (see the appendix) rather than equation (86). Making use of this formula we obtain

$$A_{kk} = \frac{\lambda^{1/2}\Gamma(1/2+|m|)}{2\sqrt{2}\pi|m|!}\,{}_3F_2\left[\begin{matrix} \frac{1}{2} & \frac{1}{2} & -k \\ 1 & 1+|m| & \end{matrix}; 1\right] \tag{87}$$

where $k = 0, 1, 2, \ldots$. When $k = 0$ (ground state for given fixed m) the value of the hypergeometric function is equal to one, and then the eigenvalues (within the first-order perturbation theory) given in equation (93) agree exactly with the variational result (141)

of section 6. Moreover, in the asymptotic limit of large $|m|$, using the Wallis' formula (Abramowitz and Stegun 1964, p 258), we obtain

$$A_{kk} \sim \frac{\lambda^{1/2}}{2\pi\sqrt{2|m|}} \qquad \text{when} \qquad |m| \to +\infty. \tag{88}$$

To see this, note that in equation (87) we have

$${}_3F_2\left[\begin{matrix}\frac{1}{2} & \frac{1}{2} & -k \\ 1 & 1+|m| & \end{matrix}; 1\right] = 1 + \sum_{s=1}^{k} \frac{\alpha_s}{g_s(|m|)}$$

where $\alpha_s \neq 0$ is a constant and $g_s(|m|) = (1+|m|)_s$ is a polynomial in $|m|$ of the degree s, as we are here using the definition $(a)_s = a(a+1)(a+2)\cdots(a+s-1)$. Therefore the expression

$${}_3F_2\left[\begin{matrix}\frac{1}{2} & \frac{1}{2} & -k \\ 1 & 1+|m| & \end{matrix}; 1\right]$$

goes to 1 for all fixed k when $|m| \to \infty$.

It is easily checked that

$$\langle x^2 \rangle = 2\pi \int_0^{+\infty} |\psi_n(x)|^2 x^3 \,\mathrm{d}x = \frac{2(1+|m|+2n)}{\lambda}. \tag{89}$$

Indeed,

$$\langle x^2 \rangle = 2\pi b_n^2 \int_0^{\infty} x^3 \,\mathrm{e}^{-\frac{\lambda}{2}x^2} x^{2|m|} \left(L_n^{|m|}\left(\frac{\lambda}{2}x^2\right)\right)^2 \mathrm{d}x. \tag{90}$$

Using the substitution $\frac{\lambda}{2}x^2 = y$, the orthogonality relation (72) and the recurrence relation of Laguerre polynomials (Abramowitz and Stegun 1964, p 783)

$$L_n^{\alpha-1}(x) = L_n^{\alpha}(x) - L_{n-1}^{\alpha}(x) \tag{91}$$

we obtain

$$\langle x^2 \rangle = \pi b_n^2 2^{|m|+2} \lambda^{-|m|-2} (|m|+1)! \left(\binom{n+|m|+1}{n} + \binom{n+|m|}{n-1}\right). \tag{92}$$

This yields equation (89); see also expression (46).

The diagonal elements A_{kk} given in equation (87) are important, because they are the first-order perturbation theory estimate of the perturbation problem (58)–(60), where the Coulomb potential energy $-2Z/x$ is treated as a small perturbation of the Landau eigenstates, and this will be a good approximation if λ is sufficiently small, and/or $|m|$ sufficiently large, namely we have

$$E_s = \epsilon_s - 4\pi Z A_{ss} \tag{93}$$

which in the asymptotic limit $|m| \gg 1$ becomes quite a simple expression, due to equation (88),

$$E_s = \epsilon_s - Z\sqrt{\frac{2\lambda}{|m|}}. \tag{94}$$

Here by E_s we denote the sth reduced dimensionless eigenvalue, so that the total dimensionless energy $\tilde{E}_s$ is given (approximated) by

$$\tilde{E}_s = \lambda(2s+|m|+m+1) - Z\sqrt{\frac{2\lambda}{|m|}} \tag{95}$$

because we have chosen $\mathrm{sign}(eB) = -1$, as $e = -e_0$, and $B > 0$, and of course $s = 0, 1, 2, \ldots$. This is a very nice and transparent result, as it shows that upon switching on the Coulomb interaction, from $Z = 0$ to $Z > 0$, we observe instead of infinitely discretely degenerate Landau levels, in fact clusters of levels, each of which has an accumulation point at precisely the Landau level. When m is negative, $m = -|m|$, but has large $|m|$, these levels approach the accumulation point as predicted in equation (95). Clearly, large $|m|$ for negative $m < 0$ leaves the Landau energy unchanged. So, the physical meaning is, because of equation (89), that we are having a charge e at a large distance from the Coulomb central charge Q in a magnetic field B, such that the (average) kinetic angular momentum l_z is also small, whilst the canonical angular momentum L_z is large. In this sense we do understand the structure of clusters of Coulomb perturbed Landau levels at large distances or large magnetic fields. In figure 1 we illustrate the structure of such Landau clusters of levels by exact numerical diagonalization of the matrix (85) for a certain range of $\lambda \in [2.5, 2.9]$.

Now we turn to a very important physical observation, which is the following. The energy spectrum of equation (58) is purely discrete for any $\lambda \neq 0$, which is clear from the shape of the potential well, which increases indefinitely for $\lambda \neq 0$ as $x \to \infty$, however small λ is. At $\lambda = 0$, i.e. in the pure Coulomb case without a magnetic field, the spectrum is discrete for all negative energies $\epsilon < 0$, has the ionization limit at $\epsilon = 0$, and the continuum at $\epsilon > 0$. What about the ionization limit in a nonvanishing magnetic field $\lambda \neq 0$, which now is not the continuum limit?

Intuitively, we would instinctively answer at the first, lowest, accumulation point. This is of course not strictly true because, at $\lambda \neq 0$, the spectrum is everywhere discrete. Nevertheless, an escape to infinity is possible. Namely, within any Landau cluster with the main quantum number fixed, according to equation (62), at negative m, but with large $|m|$, the system remains within the same cluster energetically, but with increasing $|m|$ the average radius $\langle x^2 \rangle$ is increasing linearly as given in equation (89). This is in fact nothing but almost radiationless escape to infinity, and this is what we mean by *ionization*. The photon energy needed for such escape is the smaller the larger $|m|$ is. It is in this sense that we can call the lowest Landau energy—according to equation (62) it is equal to λ—the ionization limit ϵ_{ion}. The picture somehow repeats itself then in any higher lying Landau cluster. There, ionization is possible also by emission of radiation, whilst the ionization from below ϵ_{ion} is possible by absorption of radiation, but in each case the quantum number m must change. The ionization limit thus is equal to

$$\epsilon_{\mathrm{ion}} = \lambda. \tag{96}$$

In real physical units this means, using equation (52), that the ionization limit is equal to

$$E_{\mathrm{ion}} = \frac{e_0^2}{2a_B} \times \frac{B}{B_0} = (B/B_0) \times \mathrm{Rydberg} = (B/B_0) \times 13.598\,\mathrm{eV} \tag{97}$$

where according to equation (53) $B_0 = \frac{m_e^2 e_0^3 c}{\hbar^3} = 2.3506 \times 10^9$ Gauss $= 2.3506 \times 10^5$ Tesla. As the third dimension does not change anything in this regard, the statement about the ionization limit (97) in a 3D hydrogen atom in magnetic field still holds true.

4. The representation of the Hamilton operator in the Coulomb basis

In this section we investigate the representation of our Hamilton operator (58) in the Coulomb basis, i.e. in the basis of the orthonormal discrete eigenfunctions of the 2D Coulomb problem with the general Z, sometimes also called hydrogenic basis. As is well known, this basis is *not* a complete basis in the Hilbert space, but it nevertheless plays an important role in the

perturbational analysis, where the system (58) is treated as a magnetic perturbation of the Coulomb problem, as we shall see below. This is an important approach as λ in a laboratory is always very small, $\lambda \lesssim 10^{-4}$.

We now return to equation (58) and consider the case when $\lambda = 0$, namely,

$$-\psi''(x) - \frac{\psi'(x)}{x} + \left(\frac{|m|^2}{x^2} - \frac{2Z}{x}\right)\psi(x) = \epsilon\psi(x). \tag{98}$$

The solution of interest is

$$e^{-\sqrt{-\epsilon}x} x^{|m|} {}_1F_1\left[-\frac{1}{\sqrt{-\epsilon}} + \frac{1+2|m|}{2}, 1+2|m|, 2\sqrt{-\epsilon}x\right] \tag{99}$$

because if

$$-\frac{Z}{\sqrt{-\epsilon}} + \frac{1}{2} + |m| = -n, \tag{100}$$

where $n = 0, 1, 2, \ldots$, the hypergeometric series degenerates into a polynomial, and the Schrödinger boundary conditions (71) are satisfied by the underlying solution. This implies that the eigenvalues are

$$\epsilon_n = -\frac{4Z^2}{(1+2|m|+2n)^2} \tag{101}$$

and the corresponding eigenfunctions are

$$\psi_n(x) = a_n \, \mathrm{e}^{-\frac{2Zx}{1+2|m|+2n}} x^{|m|} {}_1F_1\left[-n, 1+2|m|, \frac{4Zx}{1+2|m|+2n}\right]. \tag{102}$$

Using equation (69) we can write them in the form

$$\psi_n(x) = a_n \, \mathrm{e}^{-\frac{2Zx}{1+2|m|+2n}} x^{|m|} \frac{n!(2|m|)!}{(n+2|m|)!} L_n^{2|m|}\left(\frac{4Zx}{1+2|m|+2n}\right). \tag{103}$$

The normalization condition (71) yields

$$a_n = \frac{2^{\frac{3}{2}+2|m|}(1+2|m|+2n)^{-\frac{3}{2}-|m|}\sqrt{(2|m|+n)!}Z^{|m|+1}}{\sqrt{\pi}\,(2|m|)!\sqrt{n!}}. \tag{104}$$

Note that to compute the integral in equation (71) we used the recurrence relation for the Laguerre polynomials (91). In this way, we finally obtain the eigenfunctions

$$\psi_n(x) = \mathrm{e}^{-\frac{2Zx}{1+2|m|+2n}} x^{|m|} \frac{2^{3/2+2|m|}\sqrt{n!}Z^{|m|+1}}{\sqrt{\pi}\sqrt{(2|m|+n)!}(1+2|m|+2n)^{3/2+|m|}} L_n^{2|m|}\left(\frac{4Zx}{1+2|m|+2n}\right). \tag{105}$$

Now, denoting by $\tilde{H}$ the operator (58) with $\lambda = 0$ and by ϵ_n the eigenenergies (101) of this operator we obtain

$$H_{ks} = 2\pi \int_0^\infty x\psi_k(x)\hat{H}(\psi_s)\,\mathrm{d}x = \epsilon_s\delta_{ks} + \frac{\pi\lambda^2}{2}\int_0^\infty x^3\psi_k(x)\psi_s(x)\,\mathrm{d}x. \tag{106}$$

Using the fact that

$$L_k^{|2m|}\left(\frac{4Zx}{1+2|m|+2k}\right) L_s^{|2m|}\left(\frac{4Zx}{1+2|m|+2s}\right) = \sum_{u=0}^{k+s}\left(\sum_{j=0}^{u}(-1)^u\binom{k+2|m|}{k-j}\binom{s+2|m|}{s-u+j}\right.$$
$$\left.\times \frac{1}{j!\,(u-j)!(1+2|m|+2k)^j(1+2|m|+2s)^{u-j}}\right)(4Zx)^u \tag{107}$$

we obtain

$$A_{ks} = \int_0^{+\infty} x^3 \psi_k(x)\psi_s(x)\,\mathrm{d}x = \frac{2^{3+4|m|}(1+2k+2|m|)^{-\frac{3}{2}-|m|}(1+2|m|+2s)^{-\frac{3}{2}-|m|}\sqrt{k!}\sqrt{s!}}{\pi Z^2\sqrt{(k+2|m|)!}\sqrt{(2|m|+s)!}}$$
$$\times \sum_{u=0}^{k+s}\left(\sum_{j=0}^{u}(-1)^u\binom{k+2|m|}{k-j}\binom{s+2|m|}{s-u+j}\right.$$
$$\left.\times\frac{1}{j!\,(u-j)!(1+2|m|+2k)^j(1+2|m|+2s)^{u-j}}\right)$$
$$\times 4^u\left(\frac{(1+2k+2|m|)\,(1+2|m|+2s)}{4+4k+8|m|+4s}\right)^{4+2|m|+u}(3+2|m|+u)! \tag{108}$$

From equation (A.3) for the diagonal elements we have

$$A_{kk} = \left(\frac{a_k}{Z^{m+1}}\right)^2\frac{4^{-4-2m}(1+2k+2m)^{4+2m}k!\,(3+2m)!}{Z^2(1+2m)_k}\,{}_3F_2\left[\begin{matrix}4 & -3 & -k\\ 1 & 2|m|+1\end{matrix};1\right]$$

yielding

$$A_{kk} = \frac{(1+2k+2|m|)^2(3+5k(1+k)+5|m|+10k|m|+2|m|^2)}{16\pi Z^2}. \tag{109}$$

Again, the diagonal elements A_{kk} are important due to their role as the first-order perturbation theoretical correction of the Coulomb eigenenergies, i.e. they are the first-order analytical treatment of the quadratic Zeeman effect. The full (not reduced) eigenenergies in this approximation are, in dimensionless form, equal to

$$\tilde{\epsilon}_n = -\frac{4Z^2}{(1+2|m|+2n)^2} + m\lambda + \frac{\pi\lambda^2}{2}A_{nn} \tag{110}$$

with A_{nn} given in equation (109), which is an exact expression for the quadratic Zeeman effect. As we shall see below, for the ground state $n = 0$ of arbitrary m

$$\tilde{\epsilon}_0 = -\frac{4Z^2}{(1+2|m|)^2} + m\lambda + \frac{\lambda^2}{32Z^2}(1+2|m|)^2(3+5|m|+2|m|^2) \tag{111}$$

it exactly agrees with the variational estimates, where the latter certainly give the upper limit to the ground state.

5. The representation of the Hamilton operator in the special Landau basis $\lambda = 1$

The hydrogenic basis is (well known to be) incomplete in the Hilbert space $L^2(0, +\infty)$, whilst *the λ-Landau basis, which is the orthonormal set of the eigenfunctions of the system $\hat{H}(\lambda)$, is complete for any λ*, as demonstrated in section 3. Therefore, the hydrogenic basis can be useful at best in perturbation-like analysis of the previous section. Thus, in exact analysis the Landau basis for some λ must be used. In principle, we could use any λ-Landau basis for any $\hat{H}(\tilde{\lambda})$ system, where $\tilde{\lambda}$ is just any other value of the parameter λ, and the representation of $\hat{H}$ in the form of the matrix H_{ks} will be complete and the diagonalization of a finite dimensional approximation of this infinite matrix would formally converge to the exact value by increasing the dimensionality of the finite matrix approximant.

The question is, what λ should we choose? It seems most natural to use λ-basis for the λ-system $\hat{H}(\lambda)$. For large $\lambda \geqslant 1$ the λ-Landau basis is certainly the best for all levels. This is still true if we look at very high lying eigenstates at small λ. But at small λ, say

$\lambda \ll 1$, the λ-basis is not good, for the obvious reason that the wavelength (of oscillation) of the eigenfunctions is very large and therefore in order to describe the short-wavelength oscillations of Coulomb-like eigenfunctions we need a very large number of basis functions unlike the Coulomb-like basis analysis. The Coulomb-like eigenfunctions (i.e. slightly λ-perturbed eigenstates of the hydrogen atom) have oscillation length of order unity at low energies (but not at high energies above the zero field ionization threshold), and the same is true for the λ-basis near to $\lambda = 1$. Therefore, in exact numerical calculations of the $\hat{H}(\lambda)$ system for small $\lambda \ll 1$ and low lying states, the best method is to use the $\lambda = 1$ Landau basis. Let us now calculate this basis and the representation H_{ks} of $\hat{H}(\lambda)$ in the $(\lambda = 1)$-Landau basis.

So we now take as a basis of the Hilbert space the system of the eigenfunctions of the operator (58) without the term $2Z/x$ and with $\lambda = 1$, namely,

$$\tilde{H}(\psi) \equiv -\psi''(x) - \frac{\psi'(x)}{x} + \left(\frac{m^2}{x^2} + \frac{x^2}{4}\right)\psi(x). \tag{112}$$

Then we can write the operator (58) as

$$\hat{H}(\psi) = \tilde{H}(\psi) + \left(\frac{\lambda^2 - 1}{4}x^2 - \frac{2Z}{x}\right)\psi. \tag{113}$$

Therefore

$$H_{ks} = 2\pi \int_0^\infty x\psi_k(x)\hat{H}(\psi_s)\,\mathrm{d}x = \epsilon_s\delta_{ks} - 4\pi Z\int_0^\infty \psi_k(x)\psi_s(x)\,\mathrm{d}x + 2\pi\left(\frac{\lambda^2 - 1}{4}\right)\int_0^\infty x^3\psi_k(x)\psi_s(x)\,\mathrm{d}x \tag{114}$$

where

$$\epsilon_n = (2n + 1 + |m|) \tag{115}$$

and $n = 0, 1, 2, \ldots$. Then using equation (86) we obtain

$$D_{ks} = 4\pi\int_0^\infty \psi_k(x)\psi_s(x)\,\mathrm{d}x = \frac{\sqrt{\pi k!s!(k + |m|)!(s + |m|)!}}{2^{|m|-1}\sqrt{2}}(S_1 + S_2) \tag{116}$$

with S_1 and S_2 given by equations (83) and (84), respectively. Therefore

$$H_{ks} = -ZD_{ks} + G_{ks} \tag{117}$$

where $G = \{G_{ks}\}$ is a three-diagonal matrix defined by

$$G_{kk} = \epsilon_k + \tfrac{1}{2}(\lambda^2 - 1)(2k + |m| + 1) \tag{118}$$

$$G_{k,k+1} = -2^{|m|}\pi(\lambda^2 - 1)b_k b_{k+1}\frac{(k + |m| + 1)!}{k!} \tag{119}$$

and

$$G_{k-1,k} = -2^{|m|}\pi(\lambda^2 - 1)b_{k-1}b_k\frac{(k + |m|)!}{(k - 1)!} \tag{120}$$

where

$$b_k = \sqrt{\frac{2^{-1-|m|}}{\pi\binom{|m|+k}{k}|m|!}}. \tag{121}$$

6. Estimations and approximations of the ground state

Knowing that the ionization limit is equal to $\tilde{\epsilon}_{\rm ion} = \lambda$, as discussed and explained at the end of the section 3, see equations (96)–(97), we would like to calculate the ionization energy. For the latter, we have to know the ionization limit and the value of the ground-state energy. Perhaps this is the most important parameter and aspect of the hydrogen atom in magnetic field. Therefore, in this section we present a variety of methods to analytically estimate the value of the ground-state energy of the 2D atom in magnetic field.

6.1. The variational method

We calculate the rigorous upper bound to the eigenenergy ϵ_0 of the ground state, for any m, which is expected to be very close to the actual value, as the choice of the variational trial function is close to the exact one. Namely, we take the trial function

$$f(x) = c\,\mathrm{e}^{-\alpha x} x^{|m|} \tag{122}$$

where $\alpha > 0$ is the variational parameter, and

$$c = 2^{|m|}\sqrt{2}\alpha^{|m|+1}\Big/\sqrt{\pi\,\Gamma(2+2|m|)}. \tag{123}$$

Then

$$||f|| = \sqrt{\langle f|f\rangle} = \int_0^{+\infty} 2\pi f(x)^2 x\,\mathrm{d}x = 1 \tag{124}$$

and (see equation (58))

$$\hat{H}(f) = c\,\mathrm{e}^{-\alpha x} x^{-1+|m|}\left(-2Z + \alpha + 2|m|\alpha - x\alpha^2 + \frac{x^3\lambda^2}{4}\right). \tag{125}$$

Taking into account that

$$\int_0^{+\infty} x^{k-1}\,\mathrm{e}^{-px}\,\mathrm{d}x = \Gamma(k)/p^k \tag{126}$$

we obtain for the variational functional

$$J(\alpha, |m|) = \langle f|\hat{H}|f\rangle = j_1(\alpha, |m|) + j_2(\alpha, |m|), \tag{127}$$

where

$$j_1(\alpha, |m|) = \frac{\alpha\,(\alpha + 2\alpha|m| - 4Z)}{(1+2|m|)} \tag{128}$$

and

$$j_2(\alpha, |m|) = \frac{(1+|m|)(3+2|m|)\lambda^2}{8\alpha^2}. \tag{129}$$

The function j_1 has a global minimum equal to $-4Z^2/(1+2|m|)^2$ at the point $\alpha = 2Z/(1+2|m|)$. Therefore if λ is small we obtain the bound for the ground-state energy

$$\epsilon_0 \leqslant \min_{\alpha} J(\alpha, |m|) \leqslant -\frac{4Z^2}{(1+2|m|)^2} + \frac{(1+|m|)(1+2|m|)^2(3+2|m|)\lambda^2}{32Z^2}. \tag{130}$$

Please observe that this upper bound is in fact precisely identical to the perturbational result (111), which is quite a curious result and demonstrates the power of variational methods when the appropriate trial functions are used. For larger values of λ, the exact minimum of the variational functional $J(\alpha, |m|)$ in equation (127) must be evaluated, but the result may no longer be so excellent, as for large λ the asymptotic behaviour of the wavefunction is Gaussian $\propto \exp(-\lambda^2 x^2/4)$ rather than exponential.

6.2. Lower bound by the minimum of the potential

To obtain a rigorous lower bound for the ground-state energy, we can find the minimum of the potential

$$V(x) = \frac{m^2 - 1/4}{x^2} - \frac{2Z}{x} + \frac{\lambda^2 x^2}{4}. \tag{131}$$

However, a better approximation can be found if we consider the quadratic approximation of the potential in the point of minimum, and use the harmonic oscillator approximation of the ground state. Namely, assume that $V(x)$ reaches the minimum at the point $x = x_0$, $V(x_0) = V_{\min}$. Then we use the approximation for the potential

$$V(x) \approx V_{\min} + \frac{V''(x_0)}{2}(x - x_0)^2. \tag{132}$$

This will yield a good approximation for the ground state provided the eigenfunction is substantial in that inner area of x where the above quadratic (harmonic) approximation is good. For the Schrödinger equation

$$u''(x) + (k^2 - \mu^2 x^2)u(x) = 0 \tag{133}$$

the ground-state energy is equal to $k^2 = \mu$. Therefore, as an approximation for the ground-state energy for the potential (131) we can take

$$\epsilon_0 = V_{\min} + \sqrt{\frac{V''(x_0)}{2}}. \tag{134}$$

When $Z > 0$, $|m| > 0$ and $\lambda \approx 0$ the potential has the minimum at $x \approx \frac{-1+4|m|^2}{4Z} - \frac{\left(1-4|m|^2\right)^4\lambda^2}{1024Z^5}$,

$$V_{\min} \approx \frac{4Z^2}{1-4m^2} + \frac{(1-4m^2)^2\lambda^2}{64Z^2}. \tag{135}$$

Also at this point the second derivative of the potential is

$$V''(x_0) \approx \frac{7\lambda^2}{2} + \frac{128Z^4}{(4m^2-1)^3} \tag{136}$$

yielding the approximate quadratic harmonic approximation for the ground-state energy ϵ_0 near its potential minimum, namely, from formula (134),

$$\begin{aligned}\epsilon_0 &= V_{\min} + \sqrt{\frac{V''(x_0)}{2}} \\ &\approx \frac{4Z^2}{1-4m^2} + \frac{\left(1-4m^2\right)^2\lambda^2}{64Z^2} + \sqrt{\frac{64Z^4}{\left(4m^2-1\right)^3} + \frac{7\lambda^2}{4}}\end{aligned} \tag{137}$$

where all terms of order λ^3 or higher are omitted/neglected. For larger λ we have no explicit analytical formulae, and the ground-state energy (134) has to be evaluated numerically.

6.3. Variational method at large $\lambda \gg 1$ using the Landau trial function

Now consider the case when $\lambda \gg 1$. With the normalized (see equation (124)) Gaussian trial function, with α being the variational parameter,

$$f(x) = \frac{\mathrm{e}^{-\alpha x^2} x^{|m|}}{\sqrt{\pi}\sqrt{2^{-1-|m|}\alpha^{-1-|m|}|m|!}} \tag{138}$$

we obtain the variational functional

$$J(\alpha, |m|) = \langle f|\hat{H}|f\rangle = \frac{2^{-\frac{7}{2}}\left(-32\alpha^{\frac{3}{2}} Z\Gamma(\frac{1}{2}+|m|) + \sqrt{2}(16\alpha^2+\lambda^2)(|m|+1)!\right)}{\alpha|m|!}. \tag{139}$$

We see that for any λ the equation $J'_\alpha(\alpha, |m|) = 0$ has one real root, which for large λ is

$$\alpha \approx \frac{\lambda}{4} \tag{140}$$

yielding the upper bound for the *reduced* ground-state energy

$$E(\alpha) \approx (|m|+1)\lambda - Z\sqrt{2\lambda}\frac{\Gamma(1/2+|m|)}{|m|!} \tag{141}$$

whilst the total energy $\tilde{E}$ is $\tilde{E} = E + m\lambda$. This result is identical to the perturbational result (93) when $s = 0$ and we use equation (87). In particular, when $m = 0$,

$$\epsilon_0 \leqslant \min J(\alpha, 0) \approx \lambda - Z\sqrt{2\pi\lambda}. \tag{142}$$

Therefore, the ionization energy $I_{\text{ionization}}$, in dimensionless form, at large λ, is approximately equal to

$$I_{\text{ionization}} = \epsilon_{\text{ion}} - \epsilon_0 = Z\sqrt{2\lambda}\frac{\Gamma\left(\frac{1}{2}+|m|\right)}{|m|!} - \lambda|m| \tag{143}$$

and in the special case of $m = 0$ we have

$$I_{\text{ionization}} = \epsilon_{\text{ion}} - \epsilon_0 = Z\sqrt{2\pi\lambda}. \tag{144}$$

In the case of small λ but any m the estimate is approximately, using equation (130),

$$I_{\text{ionization}} = \lambda + \frac{4Z^2}{(1+2|m|)^2} + o(\lambda^2). \tag{145}$$

In figures 2–5 we illustrate the quality and range of our analytical approximations along with the numerical 'exact' results.

7. Semiclassical considerations and calculations

In this section we apply the leading order WKB approximation, in fact the torus quantization, to our classical Hamiltonian (19), so that we have the two torus quantized classical closed-loop action integrals equal to

$$\frac{1}{2\pi}\oint p_\varphi \,\mathrm{d}\varphi = m\hbar \qquad \frac{1}{2\pi}\oint p_\rho \,\mathrm{d}\rho = \left(n+\frac{1}{2}\right)\hbar \tag{146}$$

where $m = 0, \pm1, \pm2, \ldots$ and $n = 0, 1, 2, \ldots$ are the two integer valued quantum numbers. Now we put $e = -e_0$ and $Q = +Ze_0$, $B > 0$, hence $\text{sign}(eB) < 0$, and find

$$n + \frac{1}{2} = \frac{1}{\pi}\int_{x_1}^{x_2} \mathrm{d}x \sqrt{\epsilon - \frac{m^2}{x^2} + \frac{2Z}{x} - \frac{\lambda^2 x^2}{4}} \tag{147}$$

after using our dimensionless units introduced in section 2, as already used up to now, and also understanding that ϵ is the reduced energy, the total one being $\tilde{\epsilon} = \epsilon + m\lambda$. Here we have two real turning points $0 < x_1 < x_2 < \infty$, hence two caustics (hence the $\frac{1}{2}$ on the right-hand side of the second equation in (146) and on the left-hand side of equation (147)). The integral

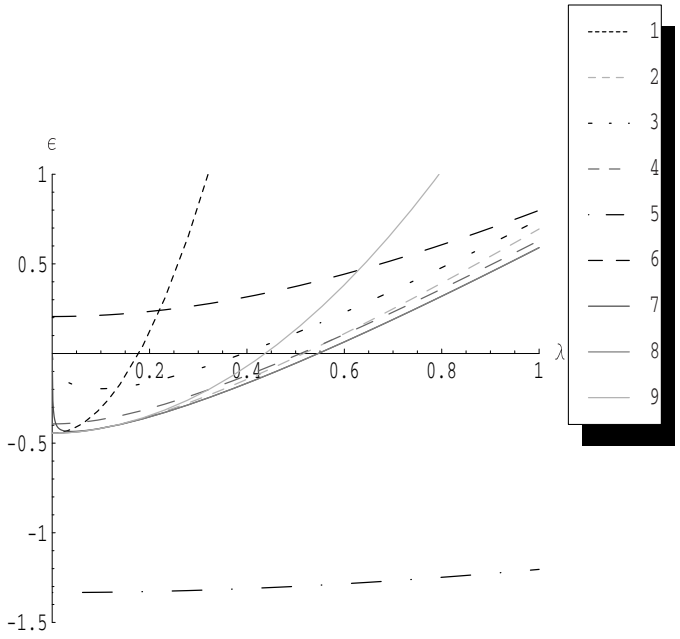

Figure 2. Estimations for the (reduced) ground-state energy in the case $m = 1$: 1, by variational method, approximation for small λ, using the Coulomb-like trial function, by formula (130); 2, by variational method, exact numerical evaluation, using the Coulomb-like trial function, by formula (127); 3, by variational method, approximation for large λ, using the Landau-like trial function, by formula (141); 4, by variational method, exact numerical evaluation, using the Landau-like trial function, by formula (139); 5, by the minimum of the potential (131), numerically evaluated—for the given range of λ it practically coincides with computing by formula (135); 6, by the harmonic oscillator ground state above the minimum of the potential, formula (134), which for the given range of λ practically coincides with (137); 7, by exact numerical results with 100×100 matrix and Landau λ-basis (70) and (85); 8, by exact numerical results with 100×100 matrix and Landau $\lambda = 1$ basis (70) and (85) with $\lambda = 1$; 9, by numerical results, diagonalization using the (incomplete) Coulomb basis, with 100×100 matrix and the Coulomb basis given (105) and (106), with (108). Note that lines 7 and 8 coincide for $\lambda \geqslant 0.06$, whilst 2,8 and 9 coincide for $\lambda \leqslant 0.2$; just above them is line 4.

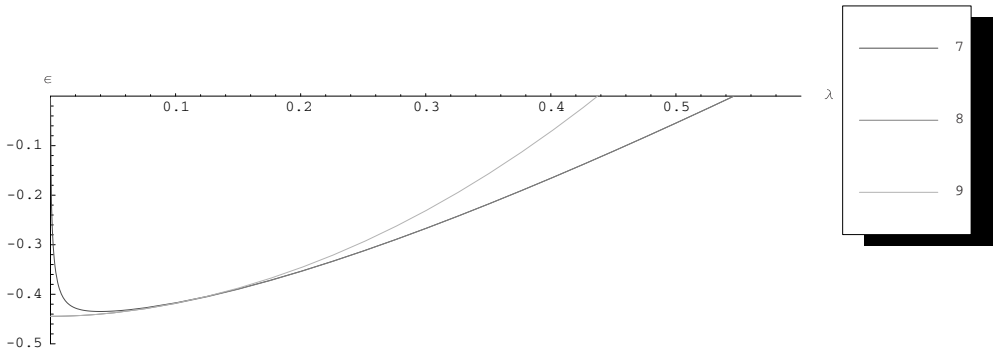

Figure 3. Lines 7, 8 and 9 of figure 2, enlarged. Lines 7 and 8 coincide when roughly $\lambda > 0.06$, line 9 is above them. We also see that lines 8 and 9 coincide for roughly $\lambda < 0.15$, which correctly matches the small λ behaviour (going to $-5/9 = 0.444\ldots$ at $\lambda = 0$).

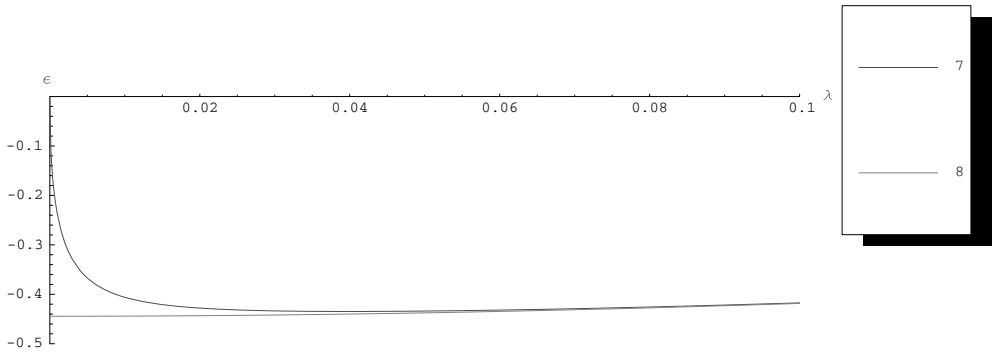

Figure 4. Lines 7 and 8 of figure 2, enlarged, in order to see the small deviations. They coincide for roughly $\lambda > 0.06$. Line 8 goes correctly to $-5/9 = 0.444\ldots$ at $\lambda = 0$, whilst line 7 fails to do so at small λ.

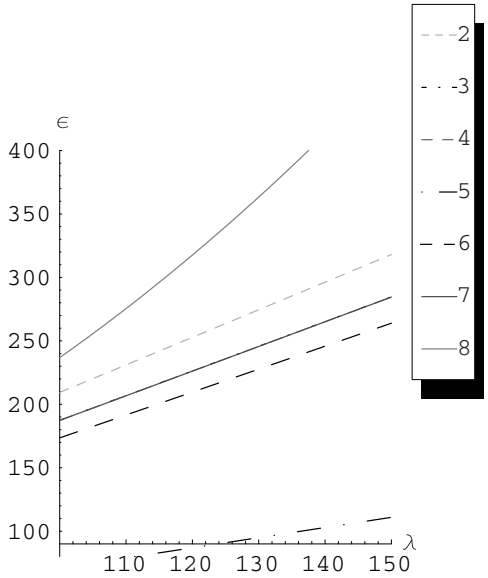

Figure 5. Estimations for the (reduced) ground-state energy for $m = 1$, for the large range of $\lambda \in [100, 150]$: 2, by variational method, exact evaluation using the Coulomb-trial function, by formula (127); 3, by variational method, approximation for large λ, using the Landau trial function, by formula (141); 4, by variational method, exact evaluation for large λ, using Landau trial function, by formula (139); 5, by the minimum of the potential (131), numerically evaluated; 6, by the ground state of the harmonic oscillator approximation above the minimum of the potential, by formula (134); 7, by exact numerical results with 100×100 matrix and Landau basis (74) and (85); 8, by exact numerical results with 100×100 matrix and Landau basis (74) with $\lambda = 1$. Note that lines 3, 4 and 7 coincide for all λ in this range. They are exact (within the graphical resolution of plotting).

is simple only in cases $\lambda = 0$ (pure Coulomb case) and $Z = 0$ (pure magnetic case). The integrals are elementary and we obtain in each case the exact reduced energy spectrum, namely

$$\epsilon = -\frac{Z^2}{\left(n + |m| + \frac{1}{2}\right)^2} \tag{148}$$

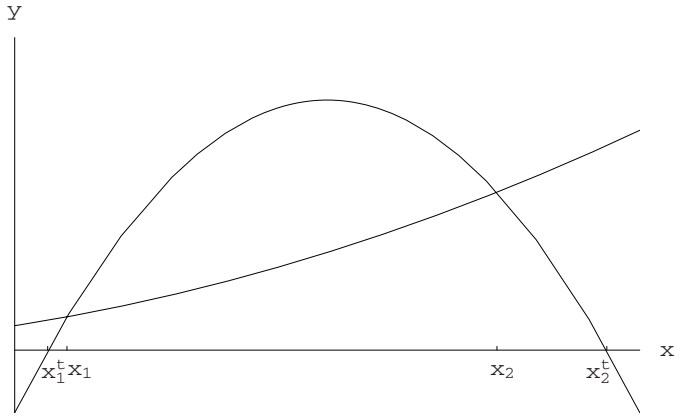

Figure 6. The turning points x_1 and x_2 as roots of the polynomial (152), as points of intersection of $y_1 = -4m^2 + 8Zx + 4\epsilon x^2$ and $y_2 = \lambda^2 x^4$. The zeros of y_1 are denoted by $x_1^t = \tilde{x}_1$ and $x_2^t = \tilde{x}_2$.

for the former and

$$\epsilon = \lambda(2n + |m| + 1) \tag{149}$$

for the latter. These results coincide with the exact results (101) and (61), respectively. Of course, the dimensionless total energy $\tilde{\epsilon} = \epsilon + m\lambda$.

The general case of the torus quantization integral (147) cannot be expressed explicitly in terms of complete elliptic integrals in an easy way, let alone in terms of elementary functions. Some results, especially for the energy level density, have been obtained by Gallas and O'Connell (1982a, 1982b), whilst the general case has not been treated analytically so far. However, instead of trying hard to express the relevant integral

$$Y = \int_{x_1}^{x_2} \frac{\mathrm{d}x}{x} \sqrt{(x - x_1)(x_2 - x)(\alpha x^2 + \beta x + \gamma)} \tag{150}$$

in terms of (complete) elliptic integrals, we shall elaborate on useful analytical approximations.

We shall denote by $N = N(\epsilon, \lambda) = Y/\pi$, which is equal to the expression in (147), and is the number of levels below the reduced energy ϵ at the given value of (the dimensionless magnetic field strength) λ, at fixed value of the angular momentum quantum number m, according to the Thomas–Fermi rule. Namely, N is equal to the classical phase space volume below ϵ divided by the 'quantum Planck cell size' $2\pi\hbar$. Thus we compute the number of levels below ϵ using the Thomas–Fermi rule

$$N(\epsilon, \lambda) = \frac{1}{\pi} \int_{x_1}^{x_2} \mathrm{d}x \sqrt{\epsilon - \frac{m^2}{x^2} + \frac{2Z}{x} - \frac{\lambda^2 x^2}{4}} = \frac{1}{2\pi} \int_{x_1}^{x_2} \mathrm{d}x \, \frac{1}{x} \sqrt{-4m^2 + 8Zx + 4\epsilon x^2 - \lambda^2 x^4} \tag{151}$$

where x_1, x_2 are the turning points, i.e. the real solutions to

$$f(x) = -4m^2 + 8Zx + 4\epsilon x^2 - \lambda^2 x^4 = 0. \tag{152}$$

When λ is small enough, $|m| > 0$ and ϵ is negative and such that $\epsilon > -Z^2/m^2$ the curves $y_1 = -4m^2 + 8Zx + 4\epsilon x^2$ and $y_2 = \lambda^2 x^4$ intersect as in figure 6, therefore $\tilde{x}_1 < x_1 < x_2 < \tilde{x}_2$, where $\tilde{x}_1 < \tilde{x}_2$ are the solutions to $-4m^2 + 8Zx + 4\epsilon x^2 = 0$. However, if λ is large, then the curves y_1 and y_2 do not intersect, which means that equation (152) has no real solutions.

To find the parametric set where the polynomial (152) has real roots, we note that when λ decreases from infinity to zero the graph of $y_2 = \lambda^2 x^4$ goes down (becomes shallower) and

at some value $\lambda = \lambda_0$ the right branch of y_1 tangents to y_2 at a point with the abscissa $x = x_0$. The point x_0 is a multiple root of $f(x)$, therefore the resultant[1] of $f(x)$ and $f'(x)$ must vanish at x_0. Computing, we obtain

$$\mathrm{Res}(f, f') = \frac{4096(4\epsilon^4 m^2 + 4\epsilon^3 Z^2 - 8\epsilon^2 m^4 \lambda^2 - 36\epsilon m^2 Z^2 \lambda^2 - 27 Z^4 \lambda^2 + 4m^6 \lambda^4)}{\lambda^{10}}.$$

The resultant vanishes for

$$\lambda_1^2 = \frac{8\epsilon^2 m^4 + 36\epsilon m^2 Z^2 + 27 Z^4 - Z(8\epsilon m^2 + 9Z^2)^{\frac{3}{2}}}{8m^6}$$

and

$$\lambda_2^2 = \frac{8\epsilon^2 m^4 + 36\epsilon m^2 Z^2 + 27 Z^4 + Z(8\epsilon m^2 + 9Z^2)^{\frac{3}{2}}}{8m^6}.$$

We denote by $g_1(\epsilon)$ and $g_2(\epsilon)$ the above numerators of λ_1^2 and λ_2^2, respectively. Then

$$g_1'(\epsilon) = 4m^2(4\epsilon m^2 + 9Z^2 - 3Z\sqrt{8\epsilon m^2 + 9Z^2})$$

and

$$g_1''(\epsilon) = 16m^4 \left(1 - \frac{3Z}{\sqrt{8\epsilon m^2 + 9Z^2}}\right)$$

hence $g_1''(\epsilon) < 0$ on $I = (-Z^2/m^2, 0)$ yielding $g_1'(\epsilon) > 0$ and $g_1(\epsilon) < 0$ on I. Similarly we can see that $g_2(\epsilon) > 0$ on I, thus equation (152) has two positive roots when $\lambda < |\lambda_2|$.

Taking into account that for $\epsilon < 0$, $m > 0$ and small λ the real roots of equation (152) are close to the solutions of

$$-4m^2 + 8Zx + 4\epsilon x^2 = 0 \tag{153}$$

that is,

$$\tilde{x}_1 = \frac{-Z + \sqrt{Z^2 + \epsilon m^2}}{\epsilon} \approx x_1 \qquad \text{and} \qquad \tilde{x}_2 = \frac{-Z - \sqrt{Z^2 + \epsilon m^2}}{\epsilon} \approx x_2 \tag{154}$$

we obtain from equation (151)

$$N(\epsilon, \lambda) \approx \frac{1}{2\pi} \int_{\tilde{x}_1}^{\tilde{x}_2} \mathrm{d}x \frac{1}{x} \sqrt{-4m^2 + 8Zx + 4\epsilon x^2} = \frac{Z}{\sqrt{-\epsilon}} - |m| \tag{155}$$

which is in fact just the Coulomb case (101) and (148).

Consider now the case $\epsilon > 0$. Obviously, if λ is large enough (curve 3 of figure 7) then the curves $y_1 = -4m^2 + 8Zx + 4\epsilon x^2$ and $y_2 = \lambda^2 x^4$ do not intersect, and, therefore, the polynomial (152) has no real roots. However, when λ decreases the branches of $y_2 = \lambda^2 x^4$ go down and at some value $\lambda = \lambda_0$ the right branch of y_1 tangents to the right branch of y_2 at some point with the abscissa $x = x_0$. As above from the resultant of f and f' we find that the curve y_1 tangents to y_2 when $\lambda = \lambda_0 = \lambda_1$ and $\lambda = \lambda_0 = \lambda_2$. Now note that for $\epsilon > 0$ we always have $\tilde{x}_2 < 0 < \tilde{x}_1$ and $|\tilde{x}_1| < |\tilde{x}_2|$. Therefore, taking into account that $\lambda_2 > \lambda_1$, from figure 7 we see that for $0 < \lambda < \lambda_2$ equation (152) has two positive roots (when $0 < \lambda < \lambda_1$ then, in addition, two negative roots appear, but they are not of interest for us).

When ϵ is positive, one positive root of $f(x)$ is

$$x_1 \approx \tilde{x}_1 = \frac{-Z + \sqrt{Z^2 + \epsilon m^2}}{\epsilon}. \tag{156}$$

[1] The resultant of two polynomials is the determinant of a certain matrix composed of their coefficients, and the two polynomials have a common zero if and only if their resultant vanishes. See e.g. (Cox *et al* 1992).

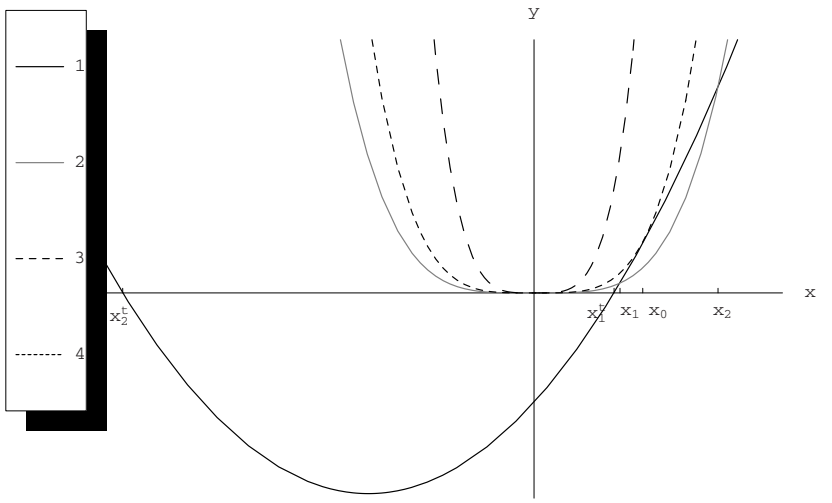

Figure 7. $x_1^t = \tilde{x}_1$ and $x_2^t = \tilde{x}_2$ are the roots of equation (153), x_1 and x_2 are the roots of (152), x_0 is the abscissa of the tangent point of (153) and $y_2 = \lambda_2^2 x^4$: 1, parabola (153) $y_1 = -4m^2 + 8Zx + 4\epsilon x^2$; 2, the graph of $y_2 = \lambda^2 x^4$ with $\lambda < \lambda_2$; 3, the graph of $y_2 = \lambda^2 x^4$ with $\lambda > \lambda_2$; 4, the graph of $y_2 = \lambda^2 x^4$ with $\lambda = \lambda_2$.

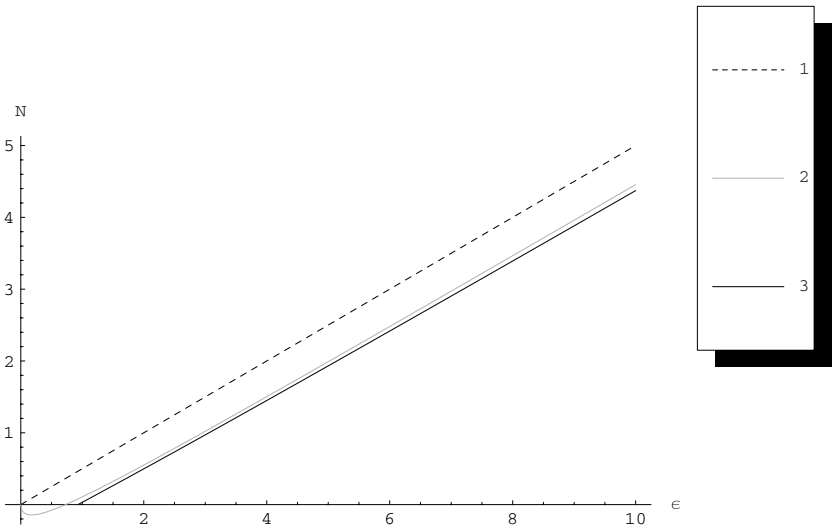

Figure 8. The function $N(\epsilon)$ for $\lambda = 1, m = 2$: 1, $N = \frac{\epsilon}{2\lambda}$; 2, by formula (157); 3, by exact numerical evaluation of integral (151).

The other is close to the root of the equation $4\epsilon x^2 - \lambda^2 x^4 = 0$, that is,

$$x_2 \approx \tilde{x}_3 = \frac{2\sqrt{\epsilon}}{\lambda}.$$

Hence, from equation (151) we obtain

$$N(\epsilon, \lambda) \approx \frac{1}{2\pi} \int_{\tilde{x}_1}^{\tilde{x}_3} \mathrm{d}x \, \frac{1}{x} \sqrt{4\epsilon x^2 - \lambda^2 x^4} \approx \frac{\epsilon}{2\lambda} + \frac{Z - \sqrt{Z^2 + m^2\epsilon}}{\pi\sqrt{\epsilon}}. \tag{157}$$

In figure 8 we show the curves (151) and (157) for $\lambda = 1$ and $m = 2$.

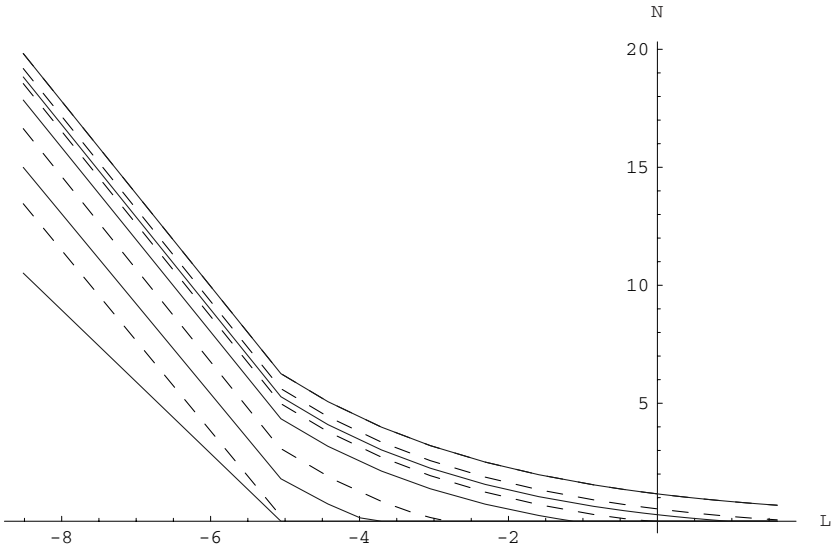

Figure 9. The function $N(\lambda)$ for $\epsilon = 0$, $m = 0, 1, 2, 5, 10$ (from top to bottom) and $Z = 1$. The dashed lines are approximations by formula (158). The full lines are exact numerical evaluations of integral (151). The abscissa is $L = \log(\lambda)$.

Consider now the case $\epsilon = 0$. In this case the roots of polynomial (152) are

$$x_1 \approx \tilde{x}_1 = \frac{m^2}{2Z} \qquad x_2 \approx \tilde{x}_4 = \frac{2Z^{1/3}}{\lambda^{2/3}}$$

and we obtain the estimation

$$N(\epsilon, \lambda) \approx \frac{1}{2\pi} \int_{\tilde{x}_1}^{\tilde{x}_4} \frac{\sqrt{8Z - \lambda^2 x^3}}{\sqrt{x}}\, \mathrm{d}x = \frac{1}{\pi} \int_{\sqrt{\tilde{x}_1}}^{\sqrt{\tilde{x}_4}} \sqrt{8Z - \lambda^2 u^6}\, \mathrm{d}u$$
$$= \frac{4Z^{2/3}}{\pi \lambda^{1/3}} \int_{\frac{\lambda^{1/3} m}{2Z^{2/3}}}^{1} \sqrt{1 - v^6}\, \mathrm{d}v = \frac{2Z^{\frac{2}{3}} \Gamma\left(\frac{7}{6}\right)}{\sqrt{\pi} \lambda^{\frac{1}{3}} \Gamma\left(\frac{5}{3}\right)} - \frac{2m_2 F_1\left(-\frac{1}{2}, \frac{1}{6}, \frac{7}{6}, \frac{m^6 \lambda^2}{64 Z^4}\right)}{\pi}. \tag{158}$$

In figure 9 we show the approximation (158) to the exact value of the integral (151), and it is seen that the quality increases with decreasing values of λ and $|m|$. In fact, for $m = 0$ the two curves overlap.

8. Discussion and conclusions

The 3D hydrogen atom in a strong magnetic field is a nonintegrable and chaotic system (Robnik 1981, 1982) which undergoes a transition from complete integrability (pure Coulomb case) to ergodicity (at sufficiently high energies). It is a generic system, having the mixed type classical phase space (Robnik 1998), and it is an example of classical (Hamiltonian) and quantum chaos *par excellence*.

The 2D hydrogen atom in a strong magnetic field is integrable and even separable, being effectively a one-dimensional system. However, its radial Schrödinger equation cannot be solved exactly. Nevertheless, much analytical work can be done. We have calculated analytically the matrix elements of the Hamilton operator in the Landau basis, which is a complete basis in the Hilbert space, and performed its numerical diagonalization, and also

described analytically the (asymptotic) structure of the Landau clusters of levels, which are created when the Coulomb interaction of an electron in a magnetic field is switched on. (If there is no Coulomb interaction, we have infinitely discretely degenerate Landau levels.) The size of the clusters scales as $\sqrt{\lambda}$ with the magnetic field strength $\lambda = B/B_0$, where $B_0 = 2.3506 \times 10^9$ G, and the levels in the cluster at fixed λ approach the accumulation point (= Landau level) as $1/\sqrt{|m|}$ when the modulus $|m|$ of the canonical angular momentum quantum number ($m = 0, \pm 1, \pm 2, \ldots$) goes to infinity (and the electron is receding to infinity). It is important that the dependence of the representation matrix (85) on magnetic field strength λ and the charge Z is known, so that it must be calculated only once. Then the eigenenergies can be obtained by a numerical diagonalization of the matrix at any desired value of λ and Z.

Moreover, we have calculated the matrix elements of the Hamilton operator in the Landau $\lambda = 1$ basis, which is better than the λ-Landau basis at small λ and negative energies (Coulomb-like regime).

Furthermore, we have calculated the representation matrix of the Hamiltonian in the *incomplete* Coulomb basis, which is useful for treatment of the small perturbations of Coulomb levels in a weak magnetic field.

We have also used the variational methods to estimate the ground state (its upper bound) and this has been done analytically for small $\lambda \ll 1$ and for large $\lambda \gg 1$. The results agree perfectly with the first-order perturbation theory in both cases. The semiclassical analysis of the problem has been outlined and the analytical approximations of the central classical action integral (within the WKB leading term) have been worked out, yielding good approximations for the density of levels.

The main conclusion is that at large values of $\lambda > 1$ we should use the λ-Landau basis, whilst for small $\lambda < 1$ and low negative energies the $\lambda = 1$ Landau basis is preferred. In each case the representation matrix of the Hamilton operator in the given basis is known analytically exact.

Acknowledgments

This work was supported by the Ministry of Education, Science and Sport of the Republic of Slovenia and by the Nova Kreditna Banka Maribor.

Appendix

The following formula for an integral containing confluent hypergeometric functions is obtained in (Landau and Lifshitz 1996, pp 666–67):

$$J_\nu = \int_0^\infty \mathrm{e}^{-kz} z^{\nu-1} [F(-n, \gamma, kz)]^2 \, \mathrm{d}z = \frac{\Gamma(\nu) n!}{k^\nu \gamma(\gamma+1)\cdots(\gamma+n-1)} \times \left(1 + \sum_{s=0}^{n-1} \frac{n(n-1\cdots(n-s)(\gamma-\nu-s-1)(\gamma-\nu-s)\cdots(\gamma-\nu+s)}{[(s+1)!]^2 \gamma(\gamma+1)\cdots(\gamma+s)}\right). \tag{A.1}$$

Applying the algorithm of Petkovšek *et al* (1996, p 36) to equation (A.1) yields

$$J_\nu = \frac{\Gamma(\nu) n!}{k^\nu (\gamma)_n} \left(1 + \frac{n(\gamma-\nu)(\gamma-\nu-1)}{\gamma} {}_4F_3 \left[\begin{matrix} 1 & 1-n & \gamma-\nu+1 & \nu-\gamma+2 \\ 2 & 2 & \gamma+1 & \end{matrix} ; 1\right]\right) \tag{A.2}$$

Taking into account the contiguous relation CO1 of the package HYP (Krattenthaler 1995),

$$ {}_{r+1}F_{s+1}\left[\begin{matrix} 1 & (A+1) \\ 2 & (B+1) \end{matrix}\ ;z\right] = \frac{\prod_{i=1}^{s} B_i}{z\prod_{i=1}^{r} A_i}\left({}_{r}F_{s}\left[\begin{matrix} (A) \\ (B) \end{matrix}\ ;z\right]-1\right) $$

we obtain from equation (A.2)

$$ J_\nu = \frac{\Gamma(\nu)n!}{k^\nu(\gamma)_n}\,{}_3F_2\left[\begin{matrix} -n & \gamma-\nu & \nu-\gamma+1 \\ 1 & \gamma & \end{matrix}\ ;1\right]. \tag{A.3} $$

References

Abramowitz M and Stegun I A 1972 *Handbook of Mathematical Functions* (New York: Dover) p 258

Blümel R and Reinhardt W P 1997 *Chaos in Atomic Physics* (Cambridge: Cambridge University Press)

Bohigas O, Giannoni M-J and Schmit C 1986 *Lecture Notes in Physics* vol 263 (Berlin: Springer) 18

Cox D, Little J and O'Shea D 1992 *Ideals, Varieties, and Algorithms* (New York: Springer-Verlag)

Friedrich H and Wintgen D 1989 *Phys. Rep.* **183** 37–79

Gallas J A C and O'Connell 1982a *J. Phys. B: At. Mol. Phys.* **15** L75

Gallas J A C and O'Connell 1982b *J. Phys. B: At. Mol. Phys.* **15** L309

Garton W R S and Tomkins F S 1969 *Astrophys. J.* **158** 839

Hasegawa H, Robnik M and Wunner G 1989 *Prog. Theor. Phys. Supp. (Kyoto)* **98** 198–286

Holle A, Main J, Wiebusch G, Rottke H and Welge K H 1988 *Phys. Rev. Lett.* **61** 161

Iu C, Welch G R, Kash M M, Kleppner D, Delande D and Gay J C 1991 *Phys. Rev. Lett.* **66** 145

Kemp J C, Swedlund J B, Landstreet J D and Angel J R P 1970 *Astrophys. J.* **161** L77

Krattenthaler C 1995 HYP and HYPQ—Mathematica packages for the manipulation of binomial sums and hypergeometric series, respectively q-binomial sums and basic hypergeometric series *J. Symbol. Comput.* **20** 737–44

Landau L D and Lifshitz E M 1997 *Quantum Mechanics* (Oxford: Butterworth-Heinemann) p 667

Mueller R O and Hughes V W 1974 *Proc. Natl. Acad. Sci. USA* **71** 3287

Petkovšek M, Wilf H S and Zeilberger D 1996 $A = B$ (Wellesley, MA: A K Peters) p 36

Robnik M 1981 *J. Phys. A: Math. Gen.* **14** 3195–216

Robnik M 1982 *J. Physique Coll.* C2 **43** 45

Robnik M 1998 *Nonlinear Phenomena in Complex Systems (Minsk)* **1** 1–22

Robnik M and Romanovski V 2002 *Nonlinear Phenomena in Complex Systems (Minsk)* **5** 445–56

Ruder H, Wunner G, Herold H and Geyer F 1994 *Atoms in Strong Magnetic Fields* (Berlin: Springer)

Stöckmann H-J 1999 *Quantum Chaos—an introduction* (Cambridge: Cambridge University Press)

Szegö G 1959 *Orthogonal Polynomials* (New York: American Mathematical Society) ch 5.7