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ETNA
Kent State University
etna@mcs.kent.edu

THE DIFFERENCE EQUATION RELATED TO THE PROBLEM OF THE HYDROGEN ATOM IN A STRONG MAGNETIC FIELD*

MARKO ROBNIK† AND VALERY G. ROMANOVSKI†

Abstract. We study the Schrödinger equation for the hydrogen atom in an 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 analytic exact solution is unknown. The problem is reduced to a linear three-term recurrence difference equation whose solution is unknown. We describe the qualitative properties of the energy spectrum and propose a semi-analytic method to numerically calculate the eigenenergies.

Key words. hydrogen atom, strong magnetic field

AMS subject classifications. 81V45, 81Q10

1. Introduction.

The problem of the hydrogen atom (or hydrogen-like atoms, or highly excited atoms - Rydberg atoms; also called planetary atoms; in the sequel we shall simply speak of the hydrogen atom) in a strong magnetic field is an important and fascinating problem [2, 4, 8, 16, 17, 21]. A first motivation comes from experimental physics, namely atomic spectroscopy, where one would like to understand the spectrum of a 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 [9] and the group of Professor Kleppner [10], although the oldest outline and suggestion for such experiments goes back to Mueller and Hughes [14]. Another phenomenon known for a long time are the quasi-Landau resonances [7]. A second motivation, perhaps even older than the laboratory experiments, comes from astrophysics, where the spectrum of the hydrogen atom in a strong magnetic field has 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 surface is 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 been finally explained in terms of the so-called stationary lines spectroscopy [24]. Theoretically it has been shown (see [21] and the 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 with respect to B at B_s vanishes (having a maximum, a minimum or an inflection there) are easily 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 stationarity condition is satisfied, and thus the estimate of the magnetic field strength in that emission region could be deduced. In a certain particular case [24] this result agreed with the determination of B through the mea-

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†CAMTP–Center for Applied Mathematics and Theoretical Physics, University of Maribor, Maribor, Krekova 2, SI-2000, Slovenia (robnik, valery.romanovsky@uni-mb.si).

surement of the circular polarization of the optical continuum by Kemp *et al.* [11], and was quite a success of the theory of atomic spectra in strong magnetic fields. The neutron stars can have polar magnetic field strengths up to $10^{13}G$, there is no hydrogen, but we can have, e.g., 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 a classical and quantal Hamiltonian nonintegrable and chaotic system [3, 4, 8, 16, 17, 22] in the 3D case. It is the example of quantum chaos *par excellence*. Indeed, the simple classical system described by the Lagrange function

$$\mathcal{L} = \frac{1}{2}m_e\mathbf{v}^2 + \frac{e}{c}\mathbf{A}\cdot\mathbf{v} - \frac{Qe}{r}, \tag{1.1}$$

where

$$\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$$

is the vector potential of a homogeneous magnetic field $\mathbf{B}$, and $\mathbf{v}$ 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, that is exhibiting a chaotic motion for certain initial conditions in the classical phase space and a regular motion on invariant tori for other initial conditions, depending on the energy, strength of the magnetic field, and on the particular initial conditions [16]. 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 strengths 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 $r = |\mathbf{r}|$. To be more precise, 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.

Let us now specialize to the 2D case $z = 0$ by rewriting the Lagrange function (1.1) in polar coordinates (ρ, ϕ),

$$\mathcal{L} = \frac{m_e}{2}(\dot\rho^2 + \rho^2\dot\varphi^2) + \frac{eB}{2c}\rho^2\dot\varphi - \frac{Qe}{\rho}. \tag{1.2}$$

After introducing the standard notation for canonical moments,

$$p_\rho = \frac{\partial\mathcal{L}}{\partial\dot\rho} = m_e\dot\rho, \quad p_\varphi = \frac{\partial\mathcal{L}}{\partial\dot\varphi} = m_e\rho^2\dot\varphi + \frac{eB}{2c}\rho^2,$$

and performing the standard procedure to construct the Hamiltonian function $\mathcal{H}$ for the system (1.2),

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

we get

$$\mathcal{H} = \frac{p_\rho^2}{2m_e} + \frac{p_\varphi^2}{2m_e\rho^2} - \frac{eBp_\varphi}{2m_ec} + \frac{e^2B^2\rho^2}{8m_ec^2} + \frac{Qe}{\rho}. \tag{1.3}$$

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

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

and, therefore,

$$\dot{\varphi} = \frac{\partial \mathcal{H}}{\partial p_\varphi} = \frac{p_\varphi}{m_e \rho^2} - \frac{eB}{2m_e c}.$$

Consequently,

$$\varphi(t) = \int_{t_0}^{t} \left(\frac{p_\varphi}{m_e \rho^2} - \frac{eB}{2m_e c}\right) dt + \varphi(t_0) \tag{1.4}$$

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 (1.3), namely

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

If we choose the coordinate system rotating at Larmor rotation frequency $\omega_L = \omega/2$ (one half cyclotron frequency!), we can eliminate in (1.2) and thus in (1.3) the paramagnetic term (linear in B), which is also clear in (1.4), getting the most simple (2-dim) form of the Hamiltonian as was proposed and studied in [16], namely

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

The *canonical angular momentum* $\mathbf{L}$ is different from the *kinetic angular momentum* $\mathbf{l}$, namely we have the definition

$$\mathbf{l} = \mathbf{r} \times m_e \mathbf{v} \tag{1.5}$$

and, thus,

$$\mathbf{l} = \mathbf{L} - \frac{e}{2c}\mathbf{r} \times (\mathbf{B} \times \mathbf{r}). \tag{1.6}$$

The z-component (parallel to $\mathbf{B}$) is equal to

$$l_z = L_z - \frac{eB}{2c}\rho^2. \tag{1.7}$$

When going over to the quantum mechanics of our problem we apply the canonical quantization rule in the ordinary coordinate space, thus replace the momentum $\mathbf{p}$ by the operator

$$\hat{\mathbf{p}} = -i\hbar\frac{\partial}{\partial \mathbf{r}}. \tag{1.8}$$

As can be verified quantum mechanically, for the angular momenta, we have precisely equation (1.6),

$$\hat{\mathbf{l}} = \hat{\mathbf{L}} - \frac{e}{2c}\mathbf{r}\times(\mathbf{B}\times\mathbf{r}). \tag{1.9}$$

In particular, the z-component is given by

$$\hat{l_z} = \hat{L_z} - \frac{eB}{2c}\rho^2$$

and has the expected value

$$< \hat{l_z} >= L_z - \frac{eB}{2c} < \rho^2 > . \tag{1.10}$$

Here $\hat{L}_z$ can be expressed in terms of polar coordinates with the polar angle φ in the form

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi} = \hat{p}_\varphi. \tag{1.11}$$

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

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_e} - \frac{eB}{2m_e c}\hat{L}_z + \frac{e^2B^2}{8m_e c^2}\rho^2 + \frac{Qe}{\rho}. \tag{1.12}$$

Using (1.8) and the polar coordinates (ρ, φ), we get the Schrödinger equation

$$\hat{H}\psi = E\psi,$$

which can be written as

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

The 3D hydrogen atom in a magnetic field is a nonintegrable and chaotic system [16], while the 2D hydrogen atom is separable (in polar coordinates) and therefore integrable. We now set up the corresponding Schrödinger equation for the 2D problem, for the separated wave function $\psi(\rho)\exp(im\varphi)$ in polar coordinates (ρ, φ), where we use the fact that $\hat{L}_z\psi = -i\hbar\frac{\partial}{\partial\varphi}\psi = m\hbar\psi$. We obtain for the radial wave function ψ,

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

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

$$\rho = a_B x, \quad a_B = \frac{\hbar^2}{m_e e_0^2}.$$

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Kent State University
etna@mcs.kent.edu

Another quantity with the dimension of length is the Landau radius

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

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

$$\tilde{\epsilon} = \frac{2a_B E}{e_0^2}. \tag{1.13}$$

Finally, the unit of magnetic field strength is

$$\lambda = (\frac{a_B}{b})^2 = B/B_0, \quad B_0 = \frac{m_e^2 e_0^3 c}{\hbar^3}. \tag{1.14}$$

For e_0 and m_e being the elementary charge and the electron's mass, respectively, we obtain

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

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

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

and after introducing the *reduced energy* ϵ,

$$\epsilon = \tilde{\epsilon} + m\lambda\,\text{sign}\,(eB),$$

we get

$$\psi'' + \frac{1}{x}\psi' + [\epsilon + \frac{2Z}{x} - \frac{m^2}{x^2} - \frac{\lambda^2}{4}x^2]\psi = 0. \tag{1.15}$$

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

2. The unresolved difference equation. We discuss the central difficulty in solving equation (1.15). Factoring the function

$$\psi(x) = x^{|m|} \exp(-\frac{\lambda x^2}{4}) w(x),$$

where $\lambda \geq 0$, we get from (1.15) the differential equation for $w(x)$,

$$w'' + w'(\frac{2|m|+1}{x} - \lambda x) + w[\tilde{\epsilon} + \lambda(m - |m| - 1) + \frac{2Z}{x}] = 0. \tag{2.1}$$

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Kent State University
etna@mcs.kent.edu

Substituting the power expansion

$$w(x) = \sum_{k=0}^{\infty} a_k x^k$$

into (2.1) with $a_1 = -2a_0/(1+2|m|)$, we obtain the three-term recursion relation

$$a_k = -\frac{2Z}{k(k+2|m|)} a_{k-1} + \frac{\lambda k - \tilde{\epsilon} - \lambda(m-|m|+1)}{k(k+2|m|)} a_{k-2}.$$

We are looking for solutions at discrete values of the eigenenergies $\tilde{\epsilon}$ that satisfy the Schrödinger integrability condition

$$2\pi \int_0^{\infty} x^{2|m|} \exp(-\frac{\lambda x^2}{2})|w(x)|^2 x dx < \infty.$$

It is not known how to determine such solutions and we raise the following question: Will $w(x)$ be a polynomial or some other function?

3. The representation of the Hamilton operator in the Landau basis. In spite of our incapability to solve the problem of the previous section, we can deduce some important analytic results. From now on, the quantum number m (the canonical angular momentum number) will be considered fixed unless stated otherwise in a explicit way. We are going to determine a solution of our problem (1.15) by finding the eigenvalues of the Hamilton operator

$$\hat{H}(\psi) \equiv -\psi''(x) - \frac{\psi'(x)}{x} + \left(\frac{m^2}{x^2} - \frac{2Z}{x} + \frac{x^2\,\lambda^2}{4}\right)\psi(x) = \tilde{H}(\psi) - \frac{2Z}{x}\psi(x), \tag{3.1}$$

where

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

Then

$$H_{ks} = 2\pi \int_0^{\infty} x\psi_k(x)\hat{H}(\psi_s)dx = \epsilon_s\delta_{ks} - 4\pi Z \int_0^{\infty} \psi_k(x)\psi_s(x)dx. \tag{3.2}$$

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

$$\epsilon_s = \lambda(2s+1+|m|), \tag{3.3}$$

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

$$\tilde{\epsilon}_s = \epsilon_s - m\lambda\,\mathrm{sign}\,(eB) = \lambda(2s+1+|m|+m), \tag{3.4}$$

because we choose sign $(eB) = -1$, as $e = -e_0$ and $B > 0$. Here $\psi_s(x)$ is the s-th (Landau) eigenfunction of $\tilde{H}$, where s is exactly the number of its nodes. Therefore to complete our task we need to diagonalize the operator $\hat{H}$, i.e., its matrix H_{ks}. This consists of three steps:

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Kent State University
etna@mcs.kent.edu

1. Show the completeness of the Landau basis of the eigenfunctions of the operator $\tilde{H}$ in the Hilbert space of all ψ radial functions. This is done below.
2. Calculate the elements of H_{ks}. This is done analytically below.
3. Diagonalize the matrix H_{ks}. This can not be done analytically, 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 (3.2) is exactly proportional to $\sqrt{\lambda}$, as it will be shown in below. This is very important, because it means that the matrix H_{ks} must be calculated analytically only once, see the equations (3.12) and (3.16), and consequently the energy spectrum can be obtained for any λ and Z by a diagonalization of (3.2). This is one of the major contributions of this paper.

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

$$\tilde{H}(\psi_s) \equiv -\psi_s''(x) - \frac{\psi_s'(x)}{x} + \left(\frac{m^2}{x^2} + \frac{x^2\,\lambda^2}{4}\right)\psi_s(x) = \epsilon_s \psi_s. \tag{3.5}$$

The substitution $y = \frac{\lambda}{2}x^2$ in equation (3.5) yields

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

This equation has a solution

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

with

$$F(a,b,z) \stackrel{def}{=} {}_1F_1\left[\begin{matrix} a \\ b \end{matrix}\,;z\right]$$

being the confluent hypergeometric function, which becomes a polynomial if

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

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

Therefore the spectrum of the equation (3.5) is precisely (3.3), where $s = 0, 1, 2, \ldots$, and the corresponding wave functions are

$$\psi_s(x) = a_s e^{-\frac{\lambda}{4}x^2} x^{|m|}\,{}_1F_1(-s, 1 + |m|, \frac{\lambda}{2}x^2). \tag{3.6}$$

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

$$L_n^{|m|}(z) = \frac{(n + |m|)!}{n!|m|!} F(-n, |m| + 1, z), \tag{3.7}$$

we can write (3.6) in the form

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

The normalizing condition

$$2\pi \int_0^{\infty} x\psi_s^2(x)dx = 1$$

and the orthogonality relation for Laguerre polynomials

$$\int_0^{+\infty} e^{-u}u^{|m|}L_n^{|m|}(u)L_k^{|m|}(u)du = \begin{cases} 0, & \text{if } n \neq k, \\ \Gamma(|m|+1)\binom{n+|m|}{n} & \text{if } n = k, \end{cases} \tag{3.8}$$

yield

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

Therefore

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

where

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

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

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

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

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

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

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

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

$$\begin{aligned} I(h) &= const\int_0^{+\infty} (e^{-y/2}y^{\alpha/2-1/4}[f(\sqrt{y}) - t(y/\lambda)])^2dy \\ &= const\int_0^{+\infty} (e^{-y}y^{\beta}[f(\sqrt{y}) - \tilde{t}(y)])^2dy < \epsilon, \end{aligned} \tag{3.9}$$

where $\beta = (2\alpha-1)/2$ and $\tilde{t}(y) = t(y/\lambda)$. Note that $h(x) \in L^2(0, +\infty)$ yields $e^{-y/2}y^{\alpha/2-1/4}$ $f(\sqrt{y}) \in L^2(0, +\infty)$. Therefore, according to Szegő [23, Chapter 5.7], there is a polynomial

ETNA
Kent State University
etna@mcs.kent.edu

$\tilde{t}(y)$ which satisfies (3.9). This completes the proof of the completeness of the Landau basis for any λ.

Now we calculate the matrix elements (3.2). One can verify that

$$L_k^{|m|}(\frac{\lambda}{2}x^2)L_s^{|m|}(\frac{\lambda}{2}x^2) = \sum_{u=0}^{k+s}\left(\sum_{j=0}^{u}\frac{(-1)^u\binom{k+|m|}{k-j}\binom{s+|m|}{s-u+j}}{j!\,(u-j)!}\right)\left(\frac{\lambda}{2}\right)^u x^{2\,u}. \tag{3.10}$$

Note that

$$\int_0^{+\infty} x^{2|m|+2u+v}e^{-\frac{\lambda}{2}x^2}dx = 2^{-\frac{1}{2}+|m|+u+\frac{v}{2}}\lambda^{-\frac{1}{2}-|m|-u-\frac{v}{2}}\Gamma(\frac{1}{2}+|m|+u+\frac{v}{2}). \tag{3.11}$$

Then, using (3.10) and (3.11) with $v=0$, we obtain

$$A_{ks} = \int_0^{\infty}\psi_k(x)\psi_s(x)dx = b_k b_s\sum_{u=0}^{k+s}\left(\sum_{j=0}^{u}\frac{(-1)^u\binom{k+|m|}{k-j}\binom{s+|m|}{s-u+j}}{j!\,(u-j)!}\right)\times \tag{3.12}$$

$$\left(\frac{\lambda}{2}\right)^u 2^{-\frac{1}{2}+|m|+u}\,\lambda^{-\frac{1}{2}-|m|-u}\,\Gamma(\frac{1}{2}+|m|+u)$$

$$= \frac{\lambda^{1/2}\sqrt{k!s!(k+|m|)!(s+|m|)!}}{2^{|m|+1}\sqrt{2\pi}}\sum_{u=0}^{k+s}\frac{(-1)^u(2|m|+2u-1)!!}{2^u}\times$$

$$\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!}.$$

To simplify the above expression, we rewrite the sum in the form

$$\sum_{u=0}^{s+k}\frac{(-1)^u(2|m|+2u-1)!!}{2^u}\times$$

$$\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!} = S_1+S_2,$$

where

$$S_1 = \sum_{u=0}^{s}\frac{(-1)^u(2|m|+2u-1)!!}{2^u}\times$$

$$\sum_{j=0}^{u}\frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!}$$

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Kent State University
etna@mcs.kent.edu

and

$$S_2 = \sum_{u=s+1}^{k+s} \frac{(-1)^u (2|m|+2u-1)!!}{2^u} \times$$

$$\sum_{j=0}^{u} \frac{1}{(|m|+j)!(k-j)!(|m|+u-j)!(s-u+j)!j!(u-j)!}$$

$$= \sum_{h=0}^{k-1} \frac{(-1)^{h+s+1}(2|m|+2h+2s+1)!!}{2^{h+s+1}} \times$$

$$\sum_{v=0}^{s} \frac{(v!)^{-1}}{(|m|+v+h+1)!(k-v-h-1)!(|m|+s-v)!(v+h+1)!(s-v)!},$$

where to get this expression for S_2 one can set $u = h+s+1$, $j = v+h+1$ and note that it suffices to consider only j between $h+1$ and $h+s+1$, because $\frac{1}{(-h-1+j)!} = 0$ for $j < h+1$.

To compute the inner sum in S_1, we write it as

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

where

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

Here we may replace the finite sum by the infinite sum because $\frac{1}{(u-j)!} = 0$ for $j > u$.

A straightforward computation yields

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

Hence, using the algorithm from [15, 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,

$$S_1 = \sum_{u=0}^{s} \frac{(-1)^u (2|m|+2u-1)!!}{2^u |m|!k!(|m|+u)!(s-u)!u!}\, {}_3F_2\left[\begin{matrix} -k & -|m|-u & -u \\ |m|+1 & s-u+1 & \end{matrix} ;-1\right]. \tag{3.13}$$

Similarly,

$$S_2 = \sum_{h=0}^{k-1} \frac{(-1)^{h+s+1}(2|m|+2h+2s+1)!!}{2^{h+s+1}(|m|+h+1)!(k-h-1)!(|m|+s)!(h+1)!s!}$$

$$\times\, {}_3F_2\left[\begin{matrix} h+1-k & -|m|-s & -s \\ h+2 & |m|+h+2 & \end{matrix} ;-1\right]. \tag{3.14}$$

As a consequence, we obtain

$$H_{ks} = \epsilon_s \delta_{ks} - 4\pi Z A_{ks}, \tag{3.15}$$

where

$$A_{ks} = \frac{\lambda^{1/2}\sqrt{k!s!(k+|m|)!(s+|m|)!}}{2^{|m|+1}\sqrt{2\pi}}\left(S_1 + S_2\right), \tag{3.16}$$

and S_1, S_2 are given by (3.13), (3.14), respectively.

Note that we have to split the sum in (3.12) into the two parts, S_1 and S_2, because otherwise, using the algorithm of [15, p. 36], we encounter the indeterminacy $0 \cdot \infty$ during the calculations.

This completes our calculation of the matrix H_{ks} representing $\hat{H}$ from (3.1) in the λ-Landau basis, as given in (3.15) - (3.16). Note that the matrix is known analytically and computable. Also the dependencies on λ and Z are explicitly known. Therefore it suffices to compute the matrix only once and then H_{ks} can be diagonalized for any λ and Z. This observation is important, because the computation of the matrix is quite CPU-time demanding.

For the diagonal elements, we get from (3.16),

$$A_{kk} = \frac{\lambda^{1/2}\Gamma(1/2+|m|)}{2\sqrt{2}\,\pi|m|!}\,{}_3F_2\left[\begin{matrix} 1/2 & 1/2 & -k \\ 1 & 1+|m| & \end{matrix}; 1\right], \tag{3.17}$$

where $k = 0, 1, 2, \ldots$. In the asymptotic limit for large $|m|$, using the Wallis's formula [1, p. 258], we obtain

$$A_{kk} \sim \frac{\lambda^{1/2}}{2\pi\sqrt{2|m|}} \text{ when } |m| \to +\infty. \tag{3.18}$$

To see this, notice that in equation (3.17) we have

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

where $\alpha_s \neq 0$ is a constant, $g_s(|m|) = (1+|m|)_s$ is a polynomial in $|m|$ of the degree s, and $(a)_s = a(a+1)(a+2)\ldots(a+s-1)$ denotes, as usual, the Pochhammer symbol. Therefore the expression

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

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

It is easily verified that

$$\langle x^2 \rangle = 2\pi \int_0^{+\infty} |\psi_n(x)|^2 x^3 dx = \frac{2(1+|m|+2n)}{\lambda}. \tag{3.19}$$

ETNA
Kent State University
etna@mcs.kent.edu

Indeed,

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

Using the substitution $\frac{\lambda}{2}x^2 = y$, the orthogonality relation (3.8), and the recurrence relation for the Laguerre polynomials [1, p. 783],

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

we obtain

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

Thus, (3.19) follows.

The diagonal elements A_{kk} given in (3.17) are important, because they are the first order perturbation estimate of the perturbation problem (3.1) - (3.2), 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. We have

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

which in the asymptotic limit $|m| \gg 1$ becomes a quite simple expression, due to (3.18),

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

Here E_s denotes the s-th reduced dimensionless eigenvalue, so that the total dimensionless energy, $\tilde{E}_s$, is given (approximated) by

$$\tilde{E}_s = \lambda(2s + |m| + m + 1) - Z\sqrt{\frac{2\lambda}{|m|}}, \tag{3.20}$$

where we have chosen sign $(eB) = -1$, as $e = -e_0$, and $B > 0$, and of course $s = 0, 1, 2, \dots$. 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, clusters of levels, each of which has an accumulation point precisely at the Landau level. When m is negative, with $|m|$ large, these levels approach the accumulation point as predicted by (3.20). Clearly, for large $|m|$, when $m < 0$, the Landau energy reamins unchanged, and the physical meaning is, because of (3.19), that we have 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, while the canonical angular momentum L_z is large. In this sense we understand the structure of clusters of Coulomb perturbed Landau levels either at large distances or large magnetic fields.

We make the following important physical observation: The energy spectrum of (3.1) is purely discrete for any $\lambda \neq 0$. This follows from the shape of the potential well, which increases indefinitely for $\lambda \neq 0$ as $x \to \infty$, even for small values of λ. For $\lambda = 0$, 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 when $\epsilon = 0$, and the continuum limit when $\epsilon > 0$.

ETNA
Kent State University
etna@mcs.kent.edu

We turn to the ionization limit in a non-vanishing magnetic field with $\lambda \neq 0$. Intuitively, one would expect this limit to be the first, lowest, accumulation point. This is of course not strictly true, because for $\lambda \neq 0$, 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 (3.4), at negative m, but with large $|m|$, the system stays within the same cluster energetically, but with increasing $|m|$ the average radius $< x^2 >$ is increasing linearly as given by equation (3.19). This is in fact nothing but almost radiationless escape to infinity, and that is what we mean by *ionization*. The photon energy needed for such an escape is smaller the larger $|m|$ is. It is in this sense that we can call the lowest Landau energy - according to (3.4) it is equal to λ - the ionization limit ϵ_{ion}. The situation is similar in any higher lying Landau cluster. There, ionization is also possible by emission of radiation, while ionization from below ϵ_{ion} is possible by absorption of radiation, but in each case the quantum number m must change. Thus, the ionization limit is equal to

$$\epsilon_{ion} = \lambda.$$

In real physical units this means, using (1.13), that the ionization limit is equal to

$$E_{ion} = \frac{e_0^2}{2a_B} \times \frac{B}{B_0} = (B/B_0) \times \text{Rydberg} = (B/B_0) \times 13.598\ \text{eV}, \tag{3.21}$$

where, according to (1.14), $B_0 = \frac{m_e^2 e_0^3 c}{\hbar^3} = 2.3506 \times 10^9$ Gauss $= 2.3506 \times 10^5$ Tesla. As the 3D situation does not change anything in this regard, the statement about the ionization limit (3.21) for a 3D hydrogen atom in a magnetic field still holds true.

4. Discussion and conclusions. The 3D hydrogen atom in a strong magnetic field is a nonintegrable and chaotic system [16, 17] undergoing a transition from complete integrability (pure Coulomb case) to ergodicity (at sufficiently high energies), being a generic system, having the mixed type classical phase space [18], 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. The essence of the problem is described in Section 2, and it boils down to a solution of a three-term recurrence relation. Nevertheless a lot of analytic 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 carried out 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 (spread) of the clusters scales as $\sqrt{\lambda}$ with the magnetic field strength $\lambda = B/B_0$, where $B_0 = 2.3506 \times 10^9$ Gauss, and the levels in the cluster for 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 to notice that the dependence of the representation matrix (3.15) in terms of the 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 for any desired values of λ and Z. Some further results and more details are published in [20].

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