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Oscillator approach to the problem of the hydrogen atom in a magnetic field and Feneuille scaling

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Abstract. An attempt has been made to derive an expression for the energy for the hydrogen atom in a uniform magnetic field having dependence on only one variable as conjectured by Feneuille. The Schrödinger equation is transformed by a complex Kustaanheimo-Stiefel transformation to that for a four-dimensional oscillator with a constraint. The equivalent oscillator problem is solved approximately to obtain an expression for the quantity n^2E (n being the principal quantum number, E the energy) as a function of a single variable $\beta_c = n^3 w_c$ (w_c being the cyclotron frequency). Agreement with experimental observations is discussed.

1. Introduction

In recent years considerable effort has been devoted by researchers to understand the problem of the hydrogen atom in a uniform magnetic field. Solution of this seemingly simple problem poses great difficulty because of the presence of the diamagnetic term which renders it non-separable. While at vanishing magnetic fields the Hamiltonian has spherical symmetry, it has cylindrical symmetry for high magnetic fields, and there exists no natural parameter capable of adiabatically changing the symmetry from spherical to cylindrical. Non-integrable systems exhibit in general irregular spectra which may be approximated in certain limiting cases by regular spectra (for a recent review in the particular context of the hydrogen atom in magnetic field see Friedrich and Wintgen (1989)). Attempts have been made to treat the problem in various semiclassical and quantal approximations by separating it into weak and strong field regimes depending on whether the value of the ratio of the diamagnetic term to the Coulomb term is small or large. Studies in the low field regime (Clark and Taylor 1982, Delos *et al* 1983, Wintgen and Friedrich 1986a, b) are helped by the separability due to the existence of an invariant (Solov'ev 1981, Herrick 1982, Gay *et al* 1983, Delande and Gay 1984; see also the recent review by Rau 1990). On the other hand, the electronic motion in the strong field regime is more or less planar and has been treated by many authors (Friedrich 1982, Greene 1983, Chu and Friedrich 1983, 1984, Friedrich and Wintgen 1985). A non-perturbative variational approach was also adopted by Smith *et al* (1972), Brandi (1975), Gallas (1984). However, these are computationally expensive and basis dependent (Zimmerman and Hullet *et al* 1983). Nevertheless all these approaches lead to valuable and interesting information regarding the energies of the electronic motion.

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A completely different but highly interesting phenomenological approach was adopted by Feneuille (1982) in which, by combining experimental and theoretical results so far obtained, he suggested that n^2E in the whole energy range might depend on only one variable $\beta_c = n^3 w_c$ (n being the principal quantum number, $w_c = eB/mc$ the cyclotron frequency, B the magnetic field strength and E the energy eigenvalue). Gallas *et al* (1983) (see also Wintgen and Friedrich 1987) showed that for high Rydberg states ($n \gg 1$) Feneuille's empirical conjecture is a direct consequence of the electronic motion in the $z = 0$ plane perpendicular to the magnetic field.

The purpose of the present paper is to report that Feneuille scaling can be achieved by treating the problem in an oscillator basis and applying various approximations. With this end in view the Schrödinger equation is transformed to an equivalent four-dimensional constrained oscillator equation by the complex Kustaanheimo-Stiefel approximation. This is done in section 2. In section 3 the energy E is derived in different approximations leading to an expression for n^2E in terms of the single variable β_c. Discussion of results and conclusions drawn are presented in section 4.

2. Hydrogen atom in uniform magnetic field as an anharmonic oscillator

The Schrödinger equation for the hydrogen atom in a uniform magnetic field of strength B in the z-direction is given by

$$\left(-\frac{\hbar^2}{2m}\nabla'^2 - \frac{e^2}{r'} + \frac{eB}{2mc}L'_z + \frac{e^2B^2}{8mc^2}(x'^2 + y'^2)\right)\Psi = \varepsilon\Psi \qquad \varepsilon < 0$$

where the paramagnetic and the diamagnetic terms are shown explicitly. Measuring energy in rydbergs, lengths in units of Bohr radius and magnetic field in units of $B_0 = m^2e^3c/\hbar^3 = 2.35 \times 10^9$ gauss, the equation reduces to

$$\left(-\nabla^2 - \frac{2}{r} + \frac{\gamma}{\hbar}L_z + \frac{\gamma^2}{4}(x^2 + y^2)\right)\Psi = E\Psi \tag{1}$$

where

$$\varepsilon = E\left(\frac{me^4}{2\hbar^2}\right) \qquad \boldsymbol{r} = \left(\frac{\hbar^2}{me^2}\right)\boldsymbol{r} \qquad B = \gamma B_0.$$

Introducing the complex form of the Kustaanheimo-Stiefel (1965) approximation (Cornish 1984) given by

$$x - iy = 2\zeta_A^*\zeta_B \qquad x + iy = 2\zeta_A\zeta_B^* \qquad z = |\zeta_A|^2 - |\zeta_B|^2$$

the Schrödinger equation (1) in the new complex variables ζ_A and ζ_B can easily be written (Bhaumik *et al* 1986) as

$$\left[\frac{\partial}{\partial\zeta_A^*}\frac{\partial}{\partial\zeta_A} + \frac{\partial}{\partial\zeta_B^*}\frac{\partial}{\partial\zeta_B} + 2 + \left(E - \frac{\gamma}{\hbar}L_z\right)(\zeta_A^*\zeta_A + \zeta_B^*\zeta_B) + \gamma^2|\zeta_A|^2|\zeta_B|^2(\zeta_A^*\zeta_A + \zeta_B^*\zeta_B)\right]\Psi = 0 \tag{2}$$

together with the constraint

$$\left(\zeta_A^*\frac{\partial}{\partial\zeta_A^*} - \zeta_A\frac{\partial}{\partial\zeta_A}\right)\Psi = -\left(\zeta_B^*\frac{\partial}{\partial\zeta_B^*} - \zeta_B\frac{\partial}{\partial\zeta_B}\right)\Psi. \tag{3}$$

The condition (3) eliminates the dependence of the actual wavefunction Ψ on the auxiliary fourth coordinate introduced through this complex mapping. A further change

of variable

$$\zeta_A = x_1 + ix_2 \qquad \zeta_B = x_3 + ix_4$$

converts equations (3) and (4) to

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}+\frac{\partial^2}{\partial x_4^2}\right)+2\left(-E+\frac{\gamma}{\hbar}L_z\right)(x_1^2+x_2^2+x_3^2+x_4^2)\right.$$
$$\left.+2\gamma^2(x_1^2+x_2^2)(x_3^2+x_4^2)(x_1^2+x_2^2+x_3^2+x_4^2)\right]\Psi = 4\Psi \tag{4}$$

and

$$\left(x_1\frac{\partial}{\partial x_2}-x_2\frac{\partial}{\partial x_1}\right)=-\left(x_3\frac{\partial}{\partial x_4}-x_4\frac{\partial}{\partial x_3}\right) \tag{5}$$

which explicitly shows the formal equivalence of the hydrogen atom in a magnetic field with the four-dimensional anharmonic oscillator with frequency $w_0 = [4((\gamma/\hbar)L_z - E)]^{1/2}$. It is to be noted that the frequency w_0 depends on L_z of the state and the latter may be replaced by the definite value $M\hbar$ corresponding to that state. The anharmonic term is of sixth order in coordinates of the four-dimensional oscillator. Furthermore, one can identify the constraint condition (5) with the L_z of the atom.

In the absence of the anharmonic term, equation (4) is a simple four-dimensional oscillator and may be solved easily (Bhaumik *et al* 1986) by the introduction of annihilation operators

$$a_\pm = \frac{1}{2}\left[\frac{(-i\,\partial/\partial x_1 + \partial/\partial x_2) - iw_0(x_1 \pm ix_2)}{\sqrt{2w_0}}\right] \tag{6a}$$

$$b_\pm = \frac{1}{2}\left[\frac{(-i\,\partial/\partial x_3 + \partial/\partial x_4) - iw_0(x_3 \pm ix_4)}{\sqrt{2w_0}}\right] \tag{6b}$$

and their Hermitian adjoints, $a_\pm^+$ and $b_\pm^+$ satisfying canonical commutation relations. If we denote the non-negative eigenvalues of $a_+^+a_+$, $a_-^+a_-$, $b_+^+b_+$ and $b_-^+b_-$ by n_+, n_-, m_+ and m_- respectively then the oscillator states can be labelled by $|n_+, n_-, m_+, m_-\rangle$. However, the constraint condition (5) (which can be identified as the z component of the angular momentum, L_z) and the principal quantum number for the hydrogen atom (for $\gamma = 0$) can be readily seen to be given by

$$\begin{aligned} n_+ - n_- &= m_- - m_+ = M \\ n_+ + m_+ + 1 &= n_- + m_- + 1 = n. \end{aligned} \tag{7}$$

Thus defining $\nu \equiv n_+ - m_+$, the states can actually be labelled by $|n, \nu, M\rangle$ instead of traditional $|n, l, m_l\rangle$. In these states we can calculate any required averages and matrix elements very easily. Thus

$$\begin{aligned} \langle x_1^2 + x_2^2\rangle &= \frac{1}{w_0}(n + \nu - M) \\ \langle x_3^2 + x_4^2\rangle &= \frac{1}{w_0}(n - \nu + M) \\ \langle (x_1^2 + x_2^2)^2\rangle &= \frac{1}{w_0^2}[\tfrac{3}{2}(n+\nu)^2 + \tfrac{1}{2} + M^2 - 3M(n+\nu)] \\ \langle (x_3^2 + x_4^2)^2\rangle &= \frac{1}{w_0^2}[\tfrac{3}{2}(n-\nu)^2 + \tfrac{1}{2} + M^2 + 3M(n-\nu)]. \end{aligned} \tag{8}$$

3. Mean-field, variational and anharmonic perturbation for energy

In this section we apply mean-field, variational and the anharmonic perturbation approximations to solve the Schrödinger equation for the four-dimensional anharmonic oscillator (4).

3.1. Mean-field approximation

To treat (4) in a mean-field approximation we approximate the anharmonic term neglecting the second- and higher-order correlations, replacing them by their averages over the oscillator states. Thus, representing expectation values by angular brackets $\langle\ \rangle$, we obtain the anharmonic term in the mean-field approximation as

$$\begin{aligned}2\gamma^2(x_1^2+x_2^2)(x_3^2+x_4^2)(x_1^2+x_2^2+x_3^2+x_4^2)&\\ =2\gamma^2[&-2\langle x_1^2+x_2^2\rangle^2\langle x_3^2+x_4^2\rangle-2\langle x_1^2+x_2^2\rangle\langle x_3^2+x_4^2\rangle^2\\ &+\{2\langle x_1^2+x_2^2\rangle\langle x_3^2+x_4^2\rangle+\langle(x_3^2+x_4^2)^2\rangle\}(x_1^2+x_2^2)\\ &+\{2\langle x_1^2+x_2^2\rangle\langle x_3^2+x_4^2\rangle+\langle(x_1^2+x_2^2)^2\rangle\}(x_3^2+x_4^2)].\end{aligned}\tag{9}$$

Substituting (9) in (4) we obtain

$$\begin{aligned}\left[\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)+\tfrac{1}{2}\Omega_m^2(x_1^2+x_2^2)\right\}+\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial x_3^2}+\frac{\partial^2}{\partial x_4^2}\right)+\tfrac{1}{2}\Omega_m'^2(x_3^2+x_4^2)\right\}\right]\Psi&\\ =(\Gamma+4)\Psi&\end{aligned}\tag{10}$$

where

$$\Omega_m^2=4\gamma^2\{2\langle x_1^2+x_2^2\rangle\langle x_3^2+x_4^2\rangle+\langle(x_3^2+x_4^2)^2\rangle\}+w_0^2\tag{11a}$$

$$\Omega_m'^2=4\gamma^2\{2\langle x_1^2+x_2^2\rangle\langle x_3^2+x_4^2\rangle+\langle(x_1^2+x_2^2)^2\rangle\}+w_0^2\tag{11b}$$

and

$$\Gamma=4\gamma^2\langle x_1^2+x_2^2\rangle\langle x_3^2+x_4^2\rangle\{\langle x_1^2+x_2^2\rangle+\langle x_3^2+x_4^2\rangle\}.\tag{11c}$$

Equation (10) can be solved to obtain an implicit equation for the energy eigenvalue $(\Gamma+4)$ in terms of Ω_m and Ω_m'. Working as before in an oscillator basis and writing the quantum numbers as n, ν and M as defined earlier, we get

$$\begin{aligned}(n+\nu-M)\Omega_m+(n-\nu+M)\Omega_m'&\\ =4\gamma^2\frac{\{n^2-(\nu-M)^2\}}{\Omega_m\Omega_m'}&\left(\frac{n+\nu-M}{\Omega_m}+\frac{n-\nu+M}{\Omega_m'}\right)+4\end{aligned}\tag{12a}$$

with

$$\Omega_m^2=w_0^2+4\gamma^2\left(\frac{2\{n^2-(\nu-M)^2\}}{\Omega_m\Omega_m'}+\frac{1}{\Omega_m'^2}\{\tfrac{3}{2}(n-\nu)^2+\tfrac{1}{2}+M^2+3M(n-\nu)\}\right)\tag{12b}$$

and

$$\Omega_m'^2 = w_0^2 + 4\gamma^2\left(\frac{2\{n^2-(\nu-M)^2\}}{\Omega_m\Omega_m'} + \frac{1}{\Omega_m^2}\{\tfrac{3}{2}(n+\nu)^2 + \tfrac{1}{2} + M^2 - 3M(n+\nu)\}\right) \tag{12c}$$

where $w_0^2 = 4(\gamma M - E)$.

Thus, in principle, solving (12*a*), (12*b*) and (12*c*), the energy E for the atom in the presence of a magnetic field can be determined in the mean field approximation. However, we are interested to obtain an expression similar to that of Feneuille (1982) where only the dependence of energy on n, the principal quantum number, is considered. For this reason we put $M = 0$, $\nu = 0$ to arrive at

$$2\Omega n = 4\gamma^2\frac{2n^3}{\Omega^3} + 4$$

where

$$\Omega_m^2 = \Omega_m'^2 \equiv \Omega^2 = -4E + \frac{4\gamma^2}{\Omega^2}(\tfrac{7}{2}n^2 + \tfrac{1}{2}).$$

These equations can be rearranged to give the energy E as a function of $w = n/\Omega$ as

$$E = -\frac{1}{2w} + \frac{5}{2}\gamma^2 w^2 + \frac{1}{2}\gamma^2\frac{w^2}{n^2} \tag{13}$$

where w is to be found from

$$4\gamma^2 w^4 + 2w - n^2 = 0. \tag{14}$$

Equations (13) and (14) are the main results of this subsection giving E as a function of w. We can give an explicit solution for E which would appear to be a function of $(n^3\gamma)$ for large n as was conjectured by Feneuille. However, we postpone writing it explicitly until we have discussed the procedure for obtaining energy from other approximations.

3.2. Variational approximations

Variational approximations can also be applied to solve equation (4) where basis states are naturally taken to be the constrained four-dimensional oscillator states with frequency Ω, assumed to be the same, for simplicity, for all the oscillator degrees of freedom. Thus minimizing the expectation value of the Hamiltonian giving rise to (4), the expectation being evaluated between the variational states $|n_+, n_-, m_+, m_-; \Omega\rangle$, we obtain an equation for Ω. This in conjunction with the eigenvalue equation can be utilized to arrive at an expression for energy. Proceeding in this manner we get (for $M = 0$, $\nu = 0$),

$$E = -\frac{1}{2w} + 3\gamma^2 w^2 + \gamma^2\frac{w^2}{n^2} \tag{15}$$

with $w = n/\Omega$ given by the equation

$$2\gamma^2 w^4\left(3 + \frac{1}{n^2}\right) + 2w - n^2 = 0. \tag{16}$$

Needless to say, the quantity n^2E scales in terms of $(n^3\gamma)$ in this case also for high Rydberg states.

3.3. Anharmonic perturbation

Instead of applying conventional perturbation theory, we use the method proposed by Halliday and Suranyi (1980) which has the virtue of fast convergence and easy computability. In our case the Hamiltonian for the Schrödinger equation (4) given by

$$H = \frac{p_1^2+p_2^2}{2} + \frac{p_3^2+p_4^2}{2} + \frac{w_0^2}{2}(x_1^2+x_2^2+x_3^2+x_4^2) + 2\gamma^2(x_1^2+x_2^2)(x_3^2+x_4^2)(x_1^2+x_2^2+x_3^2+x_4^2)$$

is rewritten in the form $H = H_0 + H_I$ where

$$H_0 = 2\gamma^2 h_1 h_2 (h_1+h_2) + \tfrac{1}{2}w_0^2(h_1+h_2) \tag{17}$$

and $H_I = H - H_0$. Here

$$h_1 = \frac{p_1^2+p_2^2}{\Omega^2} + (x_1^2+x_2^2) \tag{18a}$$

and

$$h_2 = \frac{p_3^2+p_4^2}{\Omega^2} + (x_3^2+x_4^2). \tag{18b}$$

Thus h_1 and h_2 are the two Hamiltonians for two two-dimensional oscillators, one in x_1, x_2 and the other in x_3, x_4 with frequency Ω. Equation (17) represents such oscillators raised to the third power so that the sixth-order anharmonicity in H is taken care of. Ω is at this stage an arbitrary parameter and can be determined up to desired order by demanding the termination of the perturbation correction series for the energy at a specific order. Requiring, for example, the vanishing of the first-order correction $\langle H_I \rangle = \langle H - H_0 \rangle$ we get for $M = 0$, $\nu = 0$

$$n\Omega + \frac{4E}{\Omega}n - 26\frac{\gamma^2 n^3}{\Omega^3} + 2\frac{\gamma^2 n}{\Omega^3} = 0. \tag{19a}$$

Combining this with the eigenvalue equation (for $M = 0 = \nu$)

$$n\Omega - \frac{4E}{\Omega}n + \frac{2\gamma^2 n^3}{\Omega^3}\left(3 + \frac{1}{n^2}\right) = 4 \tag{19b}$$

we can calculate the quantity n^2E for the atom as a function of n and γ occurring in the product form $(n^3\gamma)$ for large n.

3.4. 'Feneuille' scaled expression for n^2E

Calculation of energy for the atom in different approximations discussed in sections 3.1, 3.2 and 3.3 boils down to the solution of a fourth-degree polynomial equation for w

$$\zeta\gamma^2 w^4 + 2w - n^2 = 0 \tag{20}$$

and substitution of its value in the equation for energy E

$$E = -\frac{1}{2w} + \xi\gamma^2 w^2. \tag{21}$$

In equations (20) and (21) we have assumed n to be large and have introduced two parameters ξ and ζ whose values depend on the method of approximation adopted, e.g., $\xi = 3$ and $\zeta = 6$ for the variational approach of section 3.2 (cf (15) and (16)).

Solution of (20) gives

$$w = \frac{1}{2}\left(\frac{4}{\zeta}\right)^{1/3} \gamma^{-2/3} F^{1/2}[F^{-3/4}(1-F^{3/2})^{1/2} - 1] \tag{22}$$

where

$$F = \tfrac{1}{2}[\{\sqrt{(1+\tfrac{16}{27}\beta_c^2\zeta)}+1\}^{1/3} - \{\sqrt{(1+\tfrac{16}{27}\beta_c^2\zeta)}-1\}^{1/3}]$$

and $\beta_c = n^3\gamma$.

Substituting w in (21) we obtain

$$n^2E = \frac{\beta_c^{2/3}}{F^{1/2}}\left[\frac{\xi}{4}\left(\frac{4}{\zeta}\right)^{2/3}\{(1-F^{3/2})^{1/2} - F^{3/4}\}^2 - \left(\frac{\zeta}{4}\right)^{1/3} F^{3/4}\{(1-F^{3/2})^{1/2} - F^{3/4}\}^{-1}\right]. \tag{23}$$

This is the general expression for n^2E as a function of the scaling variable β_c ($= n^3\gamma$).

4. Discussion and conclusion

The expression for n^2E given by (23) contains two parameters ξ and ζ. Their values as mentioned earlier varies with the approximations used. However, taking a slightly different approach, we can determine their values by comparison with the results for the high and low field limits. Thus noting that (Feneuille 1982)

$$n^2E = -1 + \tfrac{5}{8}\beta_c^2 \qquad \text{for low field} \tag{24}$$

$$n^2E = 2\beta_c - \sqrt{2}\,\beta_c^{1/2} \qquad \text{for high field} \tag{25}$$

(where energy is measured in rydbergs) we obtain $\xi = 3.1$ and $\zeta = 2.4$. For these values of ξ and ζ the β_c value corresponding to the autoionization of the atom comes out to be 1.5 which is in good agreement with the experimental data of Gay *et al* (1980). It may be mentioned here that direct calculation of low and high β_c limits from (23) in various approximations discussed here show an apparent discrepancy with (24) and (25). For example, for low β_c equation (23) gives $\frac{3}{8}$ (instead of $\frac{5}{8}$) as the coefficient of β_c^2. This deviation can be explained by the fact that by adopting the oscillator approach to the problem we have considered essentially the 'vibrational states' for the system having $O(2)\times O(2)$ symmetry. For these states the correction to energy is $\sim\frac{3}{8}\beta_c^2$ to order β_c^2 for low β_c as was shown by Herrick (1982).

Further, to arrive at the scaling results of Feneuille we have put $M = 0$, $\gamma = 0$. The M and ν dependence of the energy complicates the analysis and no simple analytical solution for energy is possible. But it is evident from the equations for energy and frequency that for $M \neq 0$, $\nu \neq 0$, scale breaking terms appear in n^2E even for large n. This supports the conclusion drawn by Gallas *et al* (1983) that scaling reflects the dynamics of the electronic motion in the $z = 0$ plane.

In conclusion we have derived analytically an expression for the quantity n^2E exhibiting scaling in the sense that it depends on only β_c. To achieve this we have transformed the problem into an equivalent oscillator one which admits easy application of standard approximations. We believe that this oscillator approach is an extremely useful one to treat and understand similar problems of the Stark effect, the effect of crossed magnetic and electric fields, etc in an atom. We shall report the results of such analyses in the future.

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