Separability of Center of Mass and Relative Motion
of Hydrogen in Very Strong Magnetic Fields

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MASTER

Abstract

While hydrogen does not strictly separate into center of mass (CMS) and relative motion in a magnetic field, a judicious gauge choice does lead to a simple Hamiltonian whose form in a state of zero translational motion of the center of mass is that of a charged particle in a magnetic field plus a coulomb potential.

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I. Introduction

The spectrum of atomic hydrogen, long the centerpiece exercise of elementary quantum mechanics, receives recent new attention in the scientific literature.

The possibility that pulsars may have fields of the order of 10^{12} gauss has motivated much interest in the behavior of hydrogen in such enormous fields. Above 10^9 gauss the coulomb interaction on the electron will be dominated by that of the magnetic field so that the coulomb force may be treated as a perturbation to the magnetic force. Calculations of the structure and spectrum of hydrogen in such fields have been reviewed by O'Connell¹ and Garstang.²

It is noteworthy that this literature is easily accessible to students with a grasp of advanced undergraduate quantum mechanics augmented by the too often neglected problem of the charged particle in a uniform constant magnetic field. This problem, which is excellently treated elsewhere,³ is a beautiful example with which to develop the non-trivial aspects of gauge transformations on potentials and the corresponding unitary transformations on the states. Indeed, the rich degeneracy structure of the solutions, even in ground state, can hardly be interpreted without careful discussion of gauge choice and correspondingly careful distinction between canonical and mechanical momentum. A natural application of this development is then to consider hydrogen in a strong magnetic field.

The usual procedure for finding solutions to the time independent Schrodinger equation

$$H\psi = E\psi \quad (1)$$

including a strong, uniform magnetic field is to make the adiabatic approximation.⁴ For magnetic fields above 10^9 gauss the cyclotron frequency of motion in

the plane perpendicular to the field is much higher than the coulomb frequency, so that as far as the coulombic motion in the field direction is concerned the electron sees a coulomb potential averaged over the magnetic state in the perpendicular plane. The system is tightly bound in the perpendicular plane, and comparatively loosely bound in the field direction--a cigar shaped atom tending toward essentially one-dimensional coulomb motion in the field direction as the magnetic energy becomes much larger than the coulomb energy.

We take the magnetic field to lie along the z direction and use cylindrical coordinates. The adiabatic ansatz allows us to write the wave functions, ψ , as a product

$$\psi(\rho, \phi, z) = \varphi_n(\rho, \phi) f(z) \quad (2)$$

where $\varphi_n(\rho, \phi)$ is the wave function for an electron in a uniform magnetic field and $f(z)$ is to be determined. The energy levels of an electron in a magnetic field, the so called Landau levels, are given by $E_{lan} = (n + \frac{1}{2})\hbar\omega$ where $\omega = eB/m$ is the cyclotron frequency. The spacing between Landau levels is of the order of several thousand electron volts for the fields we consider so that only the $n=0$ state is treated here. Landau and Lifshitz³ give the infinitely degenerate ground state wave function as

$$\varphi_{0m}(\rho, \phi) = (\pi m!)^{-\frac{1}{2}} (\hat{\rho}^m / \hat{\rho}^{m+1}) \exp(-\rho^2 / \hat{\rho}^2) \exp(im\phi) \quad (3)$$

where $\hat{\rho} = \sqrt{2\hbar/eB}$ and $m = 0, 1, 2, 3, \dots$. Throughout this paper we will neglect spin since in the presence of a strong magnetic field it merely adds an uninteresting constant to the total energy.⁵ Past authors have invariably taken the Hamiltonian to be

$$H = \frac{1}{2m} (\vec{p} - q\vec{A})^2 - \frac{Ze^2}{4\pi\epsilon_0 r} \quad (4)$$

which is simply the Hamiltonian for a charged particle in a magnetic field plus a coulomb potential. It can be shown that (3) is an eigenfunction of the first term when $q = -e$. An equation for $f(z)$ is found by substituting the wave function (2) along with the Hamiltonian (4) into the Schrodinger equation, multiplying by φ_{00}^* , and integrating over ρ and ϕ . The resulting equation is

$$\frac{p_z^2}{2m} f(z) - \frac{Ze^2}{4\pi\epsilon_0} \int_0^\infty \int_0^\pi \frac{|\varphi_{00}|^2}{r} \rho d\rho d\phi f(z) = (E - \frac{\hbar\omega}{2}) f(z) \quad (5)$$

where the integral in the second term represents an effective coulomb potential. A summary of results from several variational calculation using (5) are given by Rau and Spruch.⁶ In a very strong magnetic field the function φ_{00} is strongly peaked near zero, approaching a delta function; in this limit we have

$$\frac{p_z^2}{2m} f(z) - \frac{Ze^2}{4\pi\epsilon_0 |z|} f(z) = (E - \frac{\hbar\omega}{2}) f(z) \quad (6)$$

or one-dimensional hydrogen, a problem whose classic references belong to this Journal.⁷

II. Separability Considerations

The use of the Hamiltonian in (4) assumes that in the center of mass system the total Hamiltonian has separated into an uninteresting center of mass piece plus the relative piece given by (4). Though the two body problem often lends itself to such a separation, the presence of an external magnetic field means that this is no longer the case. A clear exposition of the total Hamiltonian in the center of mass system does not seem to exist in the literature. In this

paper we provide such an exposition and justify the use of (4) in providing the correct energy levels for a stationary single electron atom. The total Hamiltonian must be the sum of the Hamiltonian's for each particle plus an interaction potential, thus we write

$$H = H_1 + H_2 + V_{12} \quad (7)$$

where the subscripts 1 and 2 refer to the electron and nucleus, respectively. The appropriate Hamiltonian for each particle is simply that of a charged particle in a uniform magnetic field so that

$$H = \frac{1}{2m_1} (\vec{p}_1 - q_1 \vec{A}_1)^2 + \frac{1}{2m_2} (\vec{p}_2 - q_2 \vec{A}_2)^2 + \frac{q_1 q_2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|} \quad (8)$$

where we have taken V_{12} to be the usual coulomb potential.

To proceed further with (8) we must choose the vector potentials $\vec{A}_1$ and $\vec{A}_2$ in such a manner as to preserve the manifest translation invariance of the problem. (Or see the Appendix for a more torturous route to the same result.) Since all physical results are invariant with respect to gauge transformations we have considerable freedom in our choice of vector potentials. One possible choice which possesses the same symmetry with respect to rotations about the z axis as the wave functions in (2) is

$$\vec{A}_1 = \frac{1}{c} \vec{B} \times (\vec{r}_1 - \vec{r}_2) \quad \vec{A}_2 = \frac{1}{2} \vec{B} \times (\vec{r}_2 - \vec{r}_1) \quad (9)$$

where $\vec{B}$ is the magnetic field vector. It may readily be shown that these vector potentials correctly describe the magnetic field. Substituting these vector potentials into (8) and transforming to the center of mass system by the standard transformation we find

$$\begin{aligned}
H = & \frac{\vec{P}^2}{2M} + \frac{(q_2 - q_1)}{2M} \vec{P} \cdot \vec{B} \times \vec{r} + \frac{\vec{p}^2}{2\mu} - \left(\frac{q_1}{2m_1} + \frac{q_2}{2m_2} \right) \vec{p} \cdot \vec{B} \times \vec{r} \\
& + \left(\frac{q_1^2}{8m_1} + \frac{q_2^2}{8m_2} \right) (\vec{B} \times \vec{r})^2 + \frac{q_1 q_2}{4\pi\epsilon_0 r}
\end{aligned} \tag{10}$$

where $\vec{P}$ denotes center of mass momentum, $\vec{p}$ denotes relative momentum, M is the total mass, and μ is the reduced mass. One sees immediately that the total Hamiltonian does not separate into individual center of mass and relative parts. Physically, the motion of the atom in a magnetic field produces a motional electric field, which may seen by rewriting the second term of (10) as

$$\frac{(q_2 - q_1)}{2} (\vec{P}/M \times \vec{B}) \cdot \vec{r}$$

where $\vec{P}/M \times \vec{B}$ represents an electric field as was pointed out by Lamb.⁸

We now consider the hydrogen atom as a special case, for which (10) becomes

$$\begin{aligned}
H = & \frac{\vec{P}^2}{2M} + \frac{e}{M} \vec{P} \cdot \vec{B} \times \vec{r} + \frac{\vec{p}^2}{2\mu} + \left(\frac{e}{2m_1} - \frac{e}{2m_2} \right) \vec{p} \cdot \vec{B} \times \vec{r} + \left(\frac{e^2}{8m_1} + \frac{e^2}{8m_2} \right) (\vec{B} \times \vec{r})^2 \\
& - \frac{e^2}{4\pi\epsilon_0 r}
\end{aligned} \tag{11}$$

This result is conveniently simplified if we neglect terms of order m_1/m_2 so that (11) becomes

$$H = \frac{\vec{P}^2}{2M} + \frac{e}{M} \vec{P} \cdot \vec{B} \times \vec{r} + \frac{1}{2\mu} \left(\vec{p} + \frac{e}{2} \vec{B} \times \vec{r} \right)^2 - \frac{e^2}{4\pi\epsilon_0 r} \tag{12}$$

We note that $\vec{P}$ commutes with the total Hamiltonian and hence eigenfunctions simultaneous to both $\vec{P}$ and H may be found. We write the eigenfunctions of (12) as

$$\Psi(\vec{R}, \vec{r}) = \Phi(\vec{R}) \psi_K(\vec{r}) \quad (13)$$

and require

$$\vec{P} \Phi(\vec{R}) = \vec{K} \Phi(\vec{R}) \quad (14)$$

in order that (13) be an eigenfunction of $\vec{P}$ as well as H . The continuous subscript K indicates that in general the relative Hamiltonian and hence the relative wave function will depend upon $|\vec{K}|$. The solution to (14) is simply

$$\Phi(\vec{R}) = e^{i(\vec{K} \cdot \vec{R})/\hbar} \quad (15)$$

so that the relative part of (12) becomes

$$H(\vec{p}, \vec{r}) = \frac{1}{2\mu} \left(\vec{p} + \frac{e}{2} \vec{B} \times \vec{r} \right)^2 + \frac{e}{M} \vec{K} \cdot \vec{B} \times \vec{r} - \frac{e^2}{4\pi\epsilon_0 r} \quad (16)$$

We are free to consider the stationary atom for which $\vec{K} = 0$ so that (16) reduces to (4) which confirms its validity in previous calculations.

III. Summary

In applications to astrophysics motional effects are negligible compared to the coulomb and magnetic term under consideration and the use of (4) is expected to be quite accurate. Several authors working from (4) claim that m_z , the projection of angular momentum along the z axis, is a good quantum number since L_z commutes with (4). This is not true when working with (16) since the motional electric field produces an asymmetry with respect to rotations about the z axis. However to the extent that motional effects may be neglected, this asymmetry is not expected to significantly alter previous calculations. Finally we note that the above results require that the vector potentials be invariant under translations on center of mass coordinates as was the case in (9). If this

condition is not satisfied one is not assured of finding eigenfunctions simultaneous to P and H so that the ansatz made in (15) is no longer good. The pitfalls of this approach, as well as an interesting way out, are described in the Appendix.

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Appendix

Suppose we use the gauge in which

$$\vec{A}'_1 = \frac{1}{2}(\vec{B} \times \vec{r}_1) \quad \vec{A}'_2 = \frac{1}{2}(\vec{B} \times \vec{r}_2) \quad (A1)$$

and the form of the Hamiltonian in (8). Then the Hamiltonian, expressed in terms of CM and relative coordinates in this gauge, is the ugly expression

$$\begin{aligned} H' = & \frac{\vec{P}^2}{2M} - \frac{(q_1 + q_2)}{2M} \vec{P} \cdot \vec{B} \times \vec{R} + \left[\frac{q_1^2}{8m_1} + \frac{q_2^2}{8m_2} \right] (\vec{B} \times \vec{R})^2 \\ & + \frac{(q_2 m_1 - q_1 m_2)}{2M^2} \vec{P} \cdot (\vec{B} \times \vec{r}) + \left[\frac{q_2}{2m_2} - \frac{q_1}{2m_1} \right] \vec{P} \cdot \vec{B} \times \vec{R} + \frac{1}{2m_1} \left(\vec{P} - \frac{q_1 m_2}{2M} \vec{B} \times \vec{r} \right)^2 \\ & + \frac{1}{2m_2} \left(\vec{P} - \frac{q_2 m_1}{2M} \vec{B} \times \vec{r} \right)^2 + \left[\frac{q_1^2 m_2}{4m_1 M} - \frac{q_2^2 m_1}{4m_2 M} \right] (\vec{B} \times \vec{R}) \cdot (\vec{B} \times \vec{r}) + \frac{q_1 q_2}{4\pi\epsilon_0 r} \end{aligned} \quad (A2)$$

where the partial separability is hidden because the vector potentials are not invariant with respect to translations of the center of mass. To retrieve the earlier result for the hydrogen case ($q_1 = -q_2 = -e$) let us make a unitary transformation

$$H = U H' U^\dagger$$

where

$$U = e^{i(-q_1 \vec{r}_1 - q_2 \vec{r}_2) \cdot \vec{B} \times \vec{R} / 2M} \quad (A3)$$

which induces

$$U \vec{p} U^\dagger = \vec{p} - \left(\frac{-q_1 m_2 + q_2 m_1}{2M} \right) (\vec{B} \times \vec{r})$$

$$U \vec{p} U^\dagger = \vec{p} + \left(\frac{-q_1 m_2 + q_2 m_1}{2M} \right) (\vec{B} \times \vec{R}) \quad (\text{A4})$$

and yields

$$\begin{aligned} H = & \frac{\vec{p}^2}{2M} - \frac{(q_1 + q_2)}{2M} \vec{p} \cdot \vec{B} \times \vec{R} + \frac{(q_1 + q_2)}{8M} (\vec{B} \times \vec{R})^2 + \frac{q_2 m_1 - q_1 m_2}{M^2} \vec{p} \cdot \vec{B} \times \vec{r} \\ & + \frac{-2}{2\mu} - \frac{q_1 m_2}{2m_1 M} \vec{p} \cdot \vec{B} \times \vec{r} - \frac{q_2 m_1}{2m_2 M} \vec{p} \cdot \vec{B} \times \vec{r} + \left[\frac{3(q_1 m_2 - q_2 m_1)^2}{8M^3} + \frac{q_1^2 m_2^2}{8m_1 M^2} \right. \\ & \left. + \frac{q_2^2 m_1^2}{8m_2 M^2} \right] (\vec{B} \times \vec{r})^2 + \frac{(q_1 m_2 - q_2 m_1)(q_1 + q_2)}{2M^2} (\vec{B} \times \vec{R}) \cdot (\vec{B} \times \vec{r}) + \frac{q_1 q_2}{4\pi\epsilon_0 r} \quad (\text{A5}) \end{aligned}$$

In the hydrogen case this reduces to (12). However, the unitary transformation used does not retrieve the general Hamiltonian in (10), except in the hydrogen case, $q_1 = -q_2$.

In the other cases ($q_1 \neq -q_2$) the Hamiltonian H while correct physically, is not useful because the partial separability inherent in Eq.(10) does not exist here. Conceivably there does exist a unitary transformation, not of the form (A3) which takes Eq.(A2) into Eq.(10) for the general case $q_1 \neq -q_2$.

References

1. R. F. O'Connell, Physics of Dense Matter, ed. C. J. Hansen (Dordrecht, Holland, Reidel, 1974), pp.287-300.
2. R. H. Garstang, Rep. Prog. Phys. 40, 105 (1977).
3. L. D. Landau and E. M. Lifshitz, Quantum Mechanics-Non Relativistic Theory, 2nd ed. (New York, Pergemon Press) Sec. III.
4. L. I. Schiff and H. Snyder, Phys. Rev. 55, 59 (1939).
5. M. Ruderman, Ann. Acad Sci. (NY) 257, 127 (1975).
6. A. R. P. Rau and L. Spruch, Ap. J. 207, 671 (1976).
7. R. Loudon, Am. J. Phys. 27, 649 (1959); L. Haines, D. Roberts, Am. J. Phys. 37, 1145 (1969).
8. W. E. Lamb, Phys. Rev. 85, 259 (1952).