

Hydrogen Atom in N Dimensions

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Some aspects of the N -dimensional hydrogen atom are discussed. The complete solution for the energy eigenfunctions is presented and the radial distribution function is examined. Degeneracy of energy levels, expectation values ($\langle 1/r \rangle$ and $\langle 1/r^2 \rangle$), and the virial theorem are considered. It is shown that the effect of the effective potential manifests itself in some of the aspects being investigated.

1. INTRODUCTION

Over the past decade there has been much of discussion of problems involving N dimensions. Romeo (1995) studied the Wentzel–Kramers–Brillouin (WKB) approximation in connection with hyperspherical quantum billiards. Yanez *et al.* (1994) investigated the position and momentum information entropies of N -dimensional systems. The generalization of Fermi pseudopotentials to higher dimensions was illustrated by Wo'dkiewicz (1991). Random walks and moments of inertia in N dimensions have been considered by Bender *et al.* (1994) and Bender and Mead (1995). Fukutaka and Kashiwa (1987) considered the formulation of path integrals and their quantization on N -dimensional sphere. Recently the quantization of angular momentum in N dimensions has been described by Al-Jaber (1995).

It is the purpose of this paper to investigate some aspects of the hydrogen atom in N -dimensional space. In Section 2, the energy eigenfunctions of bound states are considered. In Section 3, the radial distribution function in N dimensions is examined, and in particular the one which corresponds to the maximum value of angular momentum. In Section 4, the degeneracy of any energy level of the N -dimensional hydrogen atom is determined. In

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Section 5, the Feynman–Hellman theorem is used in order to find the expectation values $\langle 1/r \rangle$ and $\langle 1/r^2 \rangle$ and to examine the virial theorem in N dimensions.

2. ENERGY EIGENFUNCTIONS

The eigenvalue equation for a hydrogen atom is

$$\frac{-\hbar^2}{2\mu} \nabla^2 \Psi(r) - \frac{Ze^2}{r} \Psi(r) = E\Psi(r) \quad (1)$$

where μ is the reduced mass and Ze is the nuclear charge. In the N -dimensional space, the Laplacian operator in polar coordinates $(r, \theta_1, \theta_2, \dots, \theta_{N-2}, \Phi)$ of R^N is

$$\nabla^2 = r^{1-N} \frac{\partial}{\partial r} \left(r^{N-1} \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \Lambda^2 \quad (2)$$

where Λ^2 is a partial differential operator on the unit sphere S^{N-1} . Separation of variables of in equation (1) reduces it to two separate equations:

$$\Lambda^2 f + \beta f = 0 \quad (3)$$

$$r^{1-N} \frac{d}{dr} \left(r^{N-1} \frac{dR}{dr} \right) - \frac{\beta}{r^2} R + \frac{2\mu}{\hbar^2} \left(\frac{Ze^2}{r} - E \right) R = 0 \quad (4)$$

where β is a separation constant whose values (which are the eigenvalues of $-\Lambda^2$) are (Shimakura, 1992)

$$\beta = L(L + N - 2) \quad (5)$$

where $L = 0, 1, 2, \dots$

With $E < 0$ for bound states, we define ρ and λ as

$$\rho = [8\mu(-E)/\hbar^2]^{1/2} r, \quad \lambda = \left[\frac{Z^2 e^4 \mu}{2\hbar^2(-E)} \right]^{1/2}$$

and hence the radial equation for $R(\rho)$ becomes

$$\frac{d^2 R}{d\rho^2} + \frac{N-1}{\rho} \frac{dR}{d\rho} - \frac{L(L+N-2)}{\rho^2} R + \left(\frac{\lambda}{\rho} - \frac{1}{4} \right) R = 0 \quad (6)$$

We look for solutions for $R(\rho)$ in the form

$$R(\rho) = \rho^1 e^{-\rho/2} S(\rho) \quad (7)$$

The substitution of equation (7) into equation (6) yields

$$\frac{d^2S}{d\rho^2} + \left[\frac{2L + N - 1}{\rho} - 1 \right] \frac{dS}{d\rho} + \left[\frac{\lambda - L - (N - 1)/2}{\rho} \right] S = 0 \quad (8)$$

A series expansion of $S(\rho)$,

$$S(\rho) = \sum_{j=0}^{\infty} a_j \rho^j \quad (9)$$

gives us the recursion relation

$$a_{j+1} = \frac{j + L + (N - 1)/2 - \lambda}{(j + 1)(j + 2L + N - 1)} a_j \quad (10)$$

In order that the function in equation (7) have an acceptable asymptotic behavior, the series expansion of equation (9) must terminate, which means that $S(\rho)$ must be a polynomial in ρ . Let the highest power of ρ appearing in $S(\rho)$ be n_r , where $n_r = 0, 1, 2, \dots$; then the coefficient $a_{n_r + 1} = 0$, and thus the recursion formula (10) yields

$$\lambda = n_r + L + \frac{N - 1}{2} \quad (11)$$

If we introduce the principal quantum number

$$n' = n_r + L + \frac{N - 1}{2} \quad (12)$$

then equation (11) becomes

$$\lambda = n' \quad (13)$$

Comparing the associated Laguerre differential equation

$$\left[\frac{d^2}{d\rho^2} + \left(\frac{p + 1}{\rho} - 1 \right) \frac{d}{d\rho} + (q - p) \right] L_q^p(\rho) = 0 \quad (14)$$

with equation (8) gives

$$P = 2L + N - 2, \quad q = n' + L + (N - 3)/2 \quad (15)$$

The effective potential in N dimensions is (Al-Jaber, 1997)

$$V_{\text{eff}}(r) = V(r) + \left[L(L + N - 2) + \frac{(N - 1)(N - 3)}{4} \right] \frac{1}{r^2} \quad (16)$$

so if we set

$$L'(L' + 1) = L(L + N - 2) + \frac{(N - 1)(N - 3)}{4}$$

then we get

$$L' = L + \frac{N - 3}{2} \quad (17)$$

But in 3-dimensional space, the principal quantum number n is given by (Bransden and Joachain, 1989)

$$n = n_r + L + 1 \quad (18)$$

Equations (17) and (18) imply that the principal quantum number n' in N dimensions is related to that in three dimensions, n , by

$$n' = n + \frac{N - 3}{2} \quad (19)$$

and therefore (7) and (15) yield the radial solution, which is

$$R_{nL}(\rho) = A e^{-\rho/2} \rho^L L_{(n+L+N-3)}^{(2L+N-2)}(\rho) \quad (20)$$

where A is a normalization factor whose value is determined from the requirement

$$A^2 \int_0^\infty \left[e^{-\rho/2} \rho^L L_{(n+L+N-3)}^{(2L+N-2)}(\rho) \right]^2 r^{N-1} dr = 1 \quad (21)$$

Using the definition of ρ and λ and with the aid of equation (13), we get

$$\rho = \frac{2Z}{a(n + (N - 3)/2)} r \quad (22)$$

where $a (= \hbar^2/\mu e^2)$ is the Bohr radius. Hence equation (21) becomes

$$A^2 \left(\frac{a(n + (N - 3)/2)}{2Z} \right)^N \int_0^\infty e^{-\rho} \rho^{2(L+(N-3)/2)} [L_{(n+L+N-3)}^{(2L+N-2)}(\rho)]^2 \rho^2 d\rho = 1 \quad (23)$$

One should notice here that the integral in equation (23) is the one that would get if, in the corresponding integral of the three-dimensional case, L and n were replaced by $L + (N - 3)/2$ and $n + (N - 3)/2$, respectively. Therefore, equation (23) yields

$$A = \left[\left(\frac{2Z}{a(n + (N - 3)/2)} \right)^N \frac{(n - L - 1)!}{2(n + (N - 3)/2)[(n + L + N - 3)!]^3} \right]^{1/2} \quad (24)$$

Now we are in a position to write the complete energy eigenfunctions of the N -dimensional hydrogen atom, namely

$$\Psi(r, \theta_1, \theta_2, \dots, \theta_{N-2}, \phi) = AR_{nL}(r)Y_L^m(\theta_1, \theta_2, \dots, \theta_{N-2}, \phi) \quad (25)$$

where A and $R_{nL}(r)$ are given by equations (20) and (24), respectively, and $Y_L^m(\theta_1, \dots, \theta_{N-2}, \phi)$ are hyperspherical harmonics of degree L on the S^{N-1} -sphere.

The orthonormality and the addition theorem for the M linearly independent hyperspherical harmonics Y_L^m of degree L on the S^{N-1} -sphere are (Grosche and Steiner, 1995)

$$\int d\Omega Y_L^{m'}(\Omega)Y_L^m(\Omega) = \delta_{LL'} \delta_{mm'} \quad (26)$$

and

$$\sum_{m=1}^M Y_L^m(\Omega_1)Y_L^m(\Omega_2) = \frac{1}{\Omega(N)} \frac{2L + N - 2}{N - 2} C_L^{(N-2)/2}(\cos \theta_{1,2}) \quad (27)$$

Here $\Omega = \bar{X}/r$ denotes a unit vector in R^N , $\Omega(N) = 2\pi^{N/2}\Gamma(N/2)$ the volume of the N -dimensional unit sphere, and $M = (2L + N - 2)(L + N - 3)!/[L!(N - 3)!]$. The C_L^{N-2} in equation (27) are the Gegenbauer polynomials. One should notice that equation (25) reduces to the well-known energy eigenfunctions for the three-dimensional hydrogen atom when $N = 3$.

3. THE RADIAL DISTRIBUTION FUNCTION

We define the radial distribution function $D_{nL}(r)$ as

$$D_{nL}(r) = r^{N-1} |R_{nL}(r)|^2 \quad (28)$$

which gives the probability per unit length that the electron is to be found a distance r from the nucleus. The aim is to discuss the behavior of the radial distribution function when the angular momentum L has its maximum value, L_{\max} . This corresponds to $n_r = 0$ in equation (12), and using equation (19), this gives

$$L_{\max} = n' - \left(\frac{N-1}{2} \right) = n - 1 \quad (29)$$

The degree of the associated Laguerre polynomials in equation (20) when $L = L_{\max}$ is zero. In that case,

$$R_{n,n-1}(r) \sim r^{n-1} e^{-zr/a[n+(N-3)/2]} \quad (30)$$

and hence $D_{n,n-1}(r)$ will exhibit a maximum at a value of r that can be found by solving the equation

$$\frac{d}{dr} D_{n,n-1}(r) = \frac{d}{dr} \left[r^{2n+N-3} e^{-2zr/a[n+(N-3)/2]} \right] = 0$$

which gives

$$r = \frac{a}{z} \left(n + \frac{N-3}{2} \right)^2 \quad (31)$$

Now our result is straightforward. For the case $N = 3$, equation (31) reduces to the usual three-dimensional case which is found in standard quantum mechanics texts (e.g., Bransden and Joachain, 1989). For the case $N > 3$, r is larger than that of the three-dimensional result. This is due to the additional term in the effective potential [second term in brackets of equation (16)], which is repulsive in this case and hence tries to push the particle further away from the nucleus. For $N < 3$, r is smaller than the three-dimensional result. Again this is due to the additional term in the effective potential of equation (16), which is attractive in this case and hence it tries to attract the particle toward the nucleus.

4. DEGENERACY

The purpose here is to give a simple prescription for determining the degeneracy of any energy level of the hydrogen atom in N dimensions. One should recall that for any spherically symmetric potential in N dimensions (such as the one under consideration) the Schrödinger equation can be separated into an ordinary differential equation for the radial part and a partial differential equation for the angular part. The solutions to the angular part are the hyperspherical harmonics Y_L^m . If the potential has no other symmetries beyond rotational invariance, the degeneracies of energy levels are therefore the multiplicities of the hyperspherical harmonics for fixed L .

In N dimensions the hyperspherical harmonics depend on $N - 1$ angular coordinates $\theta_1, \theta_2, \dots, \theta_{N-2}, \phi$ whose ranges are $0 \leq \theta_j \leq \pi$ and $0 \leq \phi \leq 2\pi$. Each hyperspherical harmonic is determined by $N-1$ integers $L, m_1, m_2, \dots, m_{N-2}$ that can assume all values consistent with the inequalities $L \geq m_1 \geq m_2 \dots \geq |m_{N-2}| \geq 0$. On enumerating all the distinct sets of m values that are possible for a given L (taking into account both positive and negative values of m_{N-2}), one finds that the degeneracy (deg) is given by

$$\text{deg} = \sum_{l=0}^{n-1} \sum_{m_1=0}^L \sum_{m_2=0}^{m_1} \dots \sum_{-m_{N-2}}^{m_{N-2}} |m_{N-2}| \quad (32)$$

for $N > 3$ and

$$\text{deg} = \sum_{L=0}^{n-1} \sum_{\underline{L}}^{+L} |m_1| = \sum_{L=0}^{n-1} (2L + 1) = n^2 \tag{33}$$

for $N = 3$. The result of equation (33) is the known degeneracy for the three-dimensional case. The case $N=2$ needs special attention. The eigenvalues of equation (5) become, for the $N = 2$ case, L^2 and all $m_j = 0$. Therefore the degeneracy in this case is

$$\text{deg} = \sum_{-(n-1)}^{n-1} |L| = 2n - 1 \tag{34}$$

which is known from the solutions of two-dimensional problems. With the help of equations (32)–(34), results for the degeneracies of the hydrogen atom in N dimensions are given in Table I, for $N = 2$ –10 and $n = 1$ –5.

5. EXPECTATION VALUES AND VIRIAL THEOREM

Some expectation values, such as $\langle 1/r \rangle$ and $\langle 1/r^2 \rangle$, and the virial theorem for the N -dimensional hydrogen atom can be found in a direct way by applying the Feynman–Hellman theorem (Griffiths, 1995). Suppose the Hamiltonian H for a particular quantum system is a function of some parameter η ; let $E_n(\eta)$ and $\psi_n(\eta)$ be the eigenvalues and the eigenfunctions of $H(\eta)$. The Feynman–Hellman theorem states that

$$\frac{\partial E_n}{\partial \eta} = \langle \Psi_n | \frac{\partial H}{\partial \eta} | \Psi_n \rangle \tag{35}$$

The effective Hamiltonian for the radial wave functions is

Table I. Degeneracies of the Hydrogen Atom in N Dimensions ($N = 2$ –10) for Principal Quantum Number $n = 1$ –5

| | Degeneracy | | | | |
|----|------------|---------|---------|---------|---------|
| | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
| 2 | 1 | 3 | 5 | 7 | 9 |
| 3 | 1 | 4 | 9 | 16 | 25 |
| 4 | 1 | 5 | 14 | 30 | 55 |
| 5 | 1 | 6 | 20 | 50 | 105 |
| 6 | 1 | 7 | 27 | 77 | 182 |
| 7 | 1 | 8 | 35 | 112 | 294 |
| 8 | 1 | 9 | 44 | 156 | 450 |
| 9 | 1 | 10 | 54 | 210 | 665 |
| 10 | 1 | 11 | 65 | 275 | 935 |

$$H = \frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{L'(L'+1)}{r^2} - \frac{e^2}{r} \quad (36)$$

With the help of equation (17), the above effective Hamiltonian becomes

$$H = \frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu r^2} \left(L + \frac{N-3}{2} \right) \left(L + \frac{N-1}{2} \right) - \frac{e^2}{r} \quad (37)$$

The eigenvalues, using equations (12) and (19), are

$$E_n = \frac{-\mu e^4}{2\hbar^2} \frac{1}{(n_r + L + (N-1)/2)^2} \quad (38a)$$

$$= \frac{-\mu e^4}{2\hbar^2} \frac{1}{(n + (N-3)/2)^2} \quad (38b)$$

In order to find $\langle 1/r \rangle$, let the parameter $\eta = e$:

$$\frac{\partial E_n}{\partial \eta} = \frac{-2\mu e^3}{\hbar^2} \frac{1}{(n + (N-3)/2)^2}$$

$$\langle \Psi_n | \frac{\partial H}{\partial e} | \Psi_n \rangle = -2e \langle 1/r \rangle$$

and therefore the Feynman–Hellman theorem yields

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{a(n + (N-3)/2)^2} \quad (39)$$

where $a = \hbar^2/\mu e^2$.

In order to find $\langle 1/r^2 \rangle$, let the parameter $\eta = L$:

$$\frac{\partial E_n}{\partial L} = \frac{\mu e^4}{\hbar^2 (n + (N-3)/2)^3}$$

$$\langle \Psi_n | \frac{\partial H}{\partial L} | \Psi_n \rangle = \frac{\hbar^2}{2\mu} (2L + N - 2) \langle 1/r^2 \rangle$$

and hence the Feynman–Hellman theorem gives

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{a^2 (n + (N-3)/2)^3 (L + (N-3)/2)} \quad (40)$$

The expectation values given in equations (39) and (40), reduce to their counterparts in three dimensions when $N = 3$. As is also evident, these expectation values are less (greater) than the corresponding expectations in three dimensions for $N > 3$ ($N < 3$). This is again due to the extra additional

term in the effective potential, which is repulsive for $N > 3$ and attractive for $N < 3$. Finally, if we let the parameter $\eta = \mu$, then

$$\frac{\partial E_n}{\partial \mu} = \frac{1}{\mu} E_n$$

and

$$\langle \Psi_n | \frac{\partial H}{\partial \mu} | \Psi_n \rangle = -\frac{1}{\mu} \langle H - V \rangle$$

and thus the Feynman–Hellman theorem yields

$$E_n = -\langle H - V \rangle$$

which gives

$$\langle V \rangle = -2\langle T \rangle \quad (41)$$

This is the well-known virial theorem. Equation (41) shows that the virial theorem is the same in all dimensions.

6. CONCLUSION

In this paper, we have investigated some aspects of the hydrogen atom in N dimensions. The energy eigenfunctions are found and it is found that they are dimension dependent. It is shown that the effect of the effective potential, which is dimension dependent, manifests itself in some of the aspects that are considered here. We discussed the radial distribution function and in particular the one which corresponds to the maximum value of angular momentum. It is shown that the value of r at which the radial distribution function is maximum increases with N when the dimension N is greater than three and decreases with N when N is smaller than three. This is so because the effective potential becomes more repulsive when $N > 3$ and less repulsive when $N < 3$. We have also considered the degeneracy of the energy levels, which increases with the dimension N . Furthermore, with the aid of the Feynman–Hellman theorem, we have calculated the expectation values $\langle 1/r \rangle$ and $\langle 1/r^2 \rangle$, whose results are justified by the effect of the effective potential. Finally, we demonstrated that the virial theorem remains invariant when varying the dimensions N .

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