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The quantized Kepler problem

The hydrogen atom is described by a quantized Kepler problem. The resulting stationary Schrödinger equation has the form

$$\hat{H}\Psi = \Big(-\frac{\hbar^2}{2m}\Delta + \hat{V}(r)\Big)\Psi = E\Psi \qquad \hat{V}(r)\Psi = -\frac{\mu}{r}\Psi \tag{1}$$

where Δ is the Laplacian on $\mathbb{R}^3$ which in spherical coordinates becomes

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{\mathrm{S}^2} \tag{2}$$

Here Δ_{S^2}, a self-adjoint operator on $L^2(\mathrm{S}^2)$ = the Hilbert space of square-integrable functions on the sphere $L^2(\mathrm{S}^2)$, is called the *spherical Laplacian* (or, to be fancy, the *Laplace-Beltrami operator* on the manifold S^2 with its standard Riemannian metric). This operator has a discrete spectrum and a corresponding orthonormal basis of eigenfunctions, the *spherical harmonics.*

Functions on the Sphere: $\{\hat{L}_1, \hat{L}_2, \hat{L}_3\}$ acting on $L^2(\mathrm{S}^2)$

Noting that product of *commuting* Hermitian operators is Hermitian, and since $[\hat{x}_i, \hat{p}_j] = 0$ for $i \neq j$, if see that the following operators are also Hermitian:

$$\hat{L}_1 = \hat{x}_2\hat{p}_3 - \hat{x}_3\hat{p}_2 \qquad \hat{L}_2 = \hat{x}_3\hat{p}_1 - \hat{x}_1\hat{p}_3 \qquad \hat{L}_3 = \hat{x}_1\hat{p}_2 - \hat{x}_2\hat{p}_1$$

These angular momentum operators satisfy the canonical commutation relations of the Lie algebra $\mathfrak{so}(3)$

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk}\hat{L}_k \tag{3}$$

and so must generate a representation of SO(3) acting on $L^2(\mathrm{S}^2)$. This is an infinite dimensional representation, and we seek to find its irreducible components, which are all *finite dimensional.*

Introduce spherical coordinates

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{bmatrix}$$

then

$$\hat{L}_1 = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right) \quad \hat{L}_2 = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right) \quad \hat{L}_3 = -i\hbar\frac{\partial}{\partial\phi}$$

and if $\mathrm{L}^2 = \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2$ then

$$\mathrm{L}^2 = -\hbar^2\Delta_{\mathrm{S}^2} = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial^2\phi}\right)$$

One can show that L^2 commutes with all the generators L_k, and in particular

$$[\mathrm{L}^2, \hat{L}_3] = 0$$

It follows that there exists a basis of eigenfunctions in common to the commuting operators L^2 and $\hat{L}_3$. Eigenfunctions belonging to a *single* eigenvalue of L^2 span irreducible $(2\ell+1)$-dimensional representations of SO(3). Here ℓ is an integer, so all these irreducible representations are odd-dimensional. The eigenfunctions are written $Y_\ell^m(\phi,\theta)$ and satisfy the eigenvalue equations

$$\begin{aligned} \hat{L}_3 Y_\ell^m &= \hbar m Y_\ell^m \quad m = -\ell, -\ell+1, \ldots, +\ell-1, +\ell \\ \mathrm{L}^2 Y_\ell^m = -\hbar^2 \Delta_{\mathrm{S}^2} Y_\ell^m &= \hbar^2 \ell(\ell+1) Y_\ell^m \end{aligned}$$

They are simply the spherical harmonics $Y_\ell^m(\phi,\theta) = C_\ell^m e^{im\phi} P_\ell^m(\cos\theta)$, with normalization constants C_ℓ^m chosen so that Y_ℓ^m form an orthonormal basis for $L^2(\mathrm{S}^2)$:

$$\int_{S^2} Y_\ell^m Y_{\ell'}^{m'} \, dA = \delta_{\ell\ell'} \delta_{mm'}$$

Radial Dependence

Return to the stationary Schrödinger equation (1) with potential $V(r) = \mu/r$,

$$\hat{H}\Psi = \Big(-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Delta_{\mathrm{S}^2}\right) - \frac{\mu}{r}\Big)\Psi = E\Psi \tag{4}$$

we attempt to find separated solutions of the form

$$\Psi(r,\theta,\phi) = R(r)A(\theta,\phi) = \sum_{\ell,m} R_\ell^m(r) Y_\ell^m(\theta,\phi)$$

Since Y_ℓ^m are eigenfunctions of Δ_{S^2} with eigenvalue $\ell(\ell+1)$ depending only on ℓ but not on the index m, the separated radial eigenvalue equations depend only on ℓ. Assuming each ℓ-indexed equation has a discrete spectrum, we add an additional spectral index (or quantum number) k to these eigenvalue problems and write

$$-\frac{\hbar^2}{2mr^2}\Big(r^2 R_{k,\ell}'\Big)' + \frac{\hbar^2 \ell(\ell+1)}{r^2} R_{k,\ell} - \frac{\mu}{r} R_{k,\ell} = E_{k,\ell} R_{k,\ell} \tag{5}$$

This is a second order homogeneous ordinary linear differential equation with a "regular singular point" at $r = 0$. Such equations are amenable to solving by expansion techiques, having a pair of linearly independent solutions, one of which has a zero at $r = 0$, the other having a singularity at $r = 0$.

Ruling out the the singular case, we seek solutions of (5) with $R_{k,\ell}(0) = 0$ and which decay as $r \to \infty$. One can show that this happens only for discrete values of the energy, which is why we have labeled the energy with two indicies, k and ℓ. For *fixed* k and ℓ, there are $2\ell + 1$ eigenfunctions of the full hydrogen Schrödinger equation with the same radial dependence $R_{k,\ell}$, corresponding to $m = -\ell, \ldots, +\ell$.

Now the amazing thing: the energy levels $E_{k,\ell}$ depend only on the sum $n = k+\ell$. This is true only for the Coulomb potential $V(r) = \mu/r$. Instead of labeling energy with two numbers, we can label it with just n, now called the *principal quantum number*.

Fixing n, we have radial eigenfunctions $R_{n-\ell,\ell}(r)$ for $\ell = 0, 1, \ldots, n-1$, all with the same eigenvalue of energy E_n (it turns out that $E_n = \text{constant}/n^2$). So E_n is an eigenvalue of the *radial* equation of multiplicity n. However, if we lift this up to the full Schrödinger equation, each value of ℓ gives a energy level of hydrogen of multiplity $2\ell+1$. Therefore, as an eigenvalue of the hydrogen atom Schrödinger equation, E_n has multiplicity n^2:

$$\sum_{\ell=0}^{n-1} 2\ell + 1 = n^2$$

A Hidden Symmetry of the Hydrogen Atom?

In early quantum mechanics, the $(2\ell+1)$-fold degeneracy in the hydrogen atom, which we know is due to spherical SO(3)-symmetry, was called an *essential* degeneracy. But the hydrogen spectrum has n^2-fold degeneracies, so the remaining unaccounted-for degeneracies were called *accidental* degeneracies. But degeneracies in the energy spectrum indicate *symmetries* of the Hamiltonian. So what symmetry could be the source observed degeneracies of the hydrogen spectrum?

SO(4) Symmetry of the Hydrogen Atom[1]

It was already shown by Pauli in 1926 that hydrogen has a hidden SO(4)-symmetry. Like Gell-Mann with quarks, Pauli might have been led to this by noticing that SO(4) has irreducible representations of dimension n^2 (see Appendix II).

The key is to introduce a quantized version of the Laplace vector $\mathbf{A} = (A_1, A_2, A_3)$ from the classical Kepler problem. As explained in Appendix I, the components of the Laplace vector are constants of motion ("first integrals") of the Kepler problem, and so should map into three quantum mechanical observables $(\hat{A}_1, \hat{A}_2, \hat{A}_3)$ that commute with the hydrogen atom Hamiltonian:

$$[\hat{H}, \hat{A}_k] = 0 \qquad k = 1, 2, 3$$

The obervables $\hat{A}_k$ must be Hermitian operators, and the appropriate quantization of the Laplace vector is the *vector operator*

$$\mathrm{A} = (\hat{A}_1, \hat{A}_2, \hat{A}_3) = \frac{1}{2m}(\mathrm{L} \times \mathrm{p} - \mathrm{p} \times \mathrm{L}) - \frac{\mu}{|\mathrm{x}|}\mathrm{x}$$

where $\mathrm{L} = (\hat{L}_1, \hat{L}_2, \hat{L}_3)$, $\mathrm{p} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$, etc. are vector operators.

There are now some new commutation relations involving $\hat{L}_i$ and $\hat{A}_j$ that need to be computed. One set comes cheaply,

$$[\hat{L}_i, \hat{A}_j] = i\hbar\epsilon_{ijk}\hat{A}_k$$

because the Laplace vector transforms as a vector under rotation of coordinates. The next set is not so cheap:

$$[\hat{A}_i, \hat{A}_j] = i\hbar\epsilon_{ijk}\left(-\frac{2H}{m}\right)\hat{L}_k$$

Now, since $[\hat{H}, \hat{L}_k] = [\hat{H}, \hat{A}_k] = 0$ we can treat the H appearing in this equation as though it were a constant, and scale the operators $\hat{A}_k$ by setting

$$\hat{M}_k = \sqrt{\frac{m}{-2H}}\hat{A}_k$$

When this is done we have, finally, the following set of commutation relations

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k \quad [\hat{L}_i, \hat{M}_j] = i\hbar\epsilon_{ijk}\hat{M}_k \quad [\hat{M}_i, \hat{M}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$$

These commutation relations match the defining commutation relations of SO(4) (Appendix II, Equation 9)

[1] I borrow heavily from A.Zee, "Group Theory in a Nutshell for Physicists", Chapter VII.i1

Appendix I: Laplace Vector in the Kepler Problem

Reference: This topic has an excellent wiki page, which also discusses quantum mechanics of the hydrogen atom. Here's a link:
https://en.wikipedia.org/wiki/Laplace%E2%80%93Runge%E2%80%93Lenz_vector

A quick sketch of how this works. We write the fundamental constants of motion for the planar Kepler problem in the form

$$-\frac{\mu}{2a} = \frac{1}{2}|\mathbf{p}|^2 - \frac{\mu}{|\mathbf{x}|} \quad (6)$$

$$a(1-e^2) = \frac{|\mathbf{L}|^2}{\mu} \quad (7)$$

Equation (6) gives total energy, here taken to be negative implying bounded elliptical orbits. $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ is angular momentum, a is the semimajor axis, and e is orbital eccentricity. We observe that

$$\begin{aligned} \frac{d}{dt}(\mathbf{p} \times \mathbf{L}) &= -\frac{\mu}{|\mathbf{x}|^3}\, \mathbf{x} \times (\mathbf{x} \times \mathbf{p}) \\ &= \frac{\mu}{|\mathbf{x}|}\left(\mathrm{I} - \mathbf{u}_q \mathbf{u}_q^{\mathrm{T}}\right)\mathbf{p} \\ &= \mu \frac{d}{dt}\mathbf{u}_q \end{aligned}$$

where $\mathbf{u}_q = \mathbf{x}/|\mathbf{x}|$. Hence

$$\mathbf{A} = \frac{1}{\mu}(\mathbf{p} \times \mathbf{L}) - \mathbf{u}_q = \mathit{constant} \quad (8)$$

$\mathbf{A}$, a constant vector, is called the *Laplace vector* (or the Laplace-Runge-Lenz vector). It has magnitude e (and so vanishes for circular orbits), lies in the orbital plane, and when $e > 0$ is directed at perigee. To see this, we compute

$$\begin{aligned} |\mathbf{A}|^2 &= \frac{1}{\mu^2}|\mathbf{p} \times \mathbf{L}|^2 - \frac{2}{\mu}\mathbf{u}_q^{\mathrm{T}}(\mathbf{p} \times \mathbf{L}) + 1 \\ &= \frac{1}{\mu^2}|\mathbf{p}|^2|\mathbf{L}|^2 - \frac{2}{\mu|\mathbf{x}|}\, \mathbf{x}^{\mathrm{T}}(\mathbf{p} \times \mathbf{L}) + 1 \\ &= \frac{1}{\mu^2}|\mathbf{p}|^2|\mathbf{L}|^2 - \frac{2}{\mu|\mathbf{x}|}\, |\mathbf{L}|^2 + 1 \\ &= \frac{2p}{\mu}\left(\frac{1}{2}|\mathbf{p}|^2 - \frac{\mu}{|\mathbf{x}|}\right) + 1 \\ &= e^2 \end{aligned}$$

using (6) and (7). Because $\mathbf{p}$ has no radial component at perigee and apogee, one sees from (8) that $\mathbf{A}$, being constant, must be directed either toward perigee or toward apogee. In other words, $\mathbf{A}$ lies along the line of apsides. But one finds that at perigee

$$\mathbf{x}^{\mathrm{T}}\mathbf{A} > 0$$

showing that $\mathbf{A}$ is directed toward perigee. Since $\mathbf{A}$ is constant, orbits of the Kepler problem have a fixed perigee (no precession of perigee). This implies that all orbits (of negative energy) are closed, a property belonging exclusively to bound orbits of the $1/r$ potential.

Appendix II: Representations of SO(4) and its Lie Algebra $\mathfrak{so}(4)$

The Lie group SO(4) is 6-dimensional. Just as in the case of rotations of 3-space, the Lie algebra $\mathfrak{so}(4)$ is conveniently represented as the algebra of skew-symmetric 4×4 matrices under commutation.

It is easy to write down a basis. Define the following 6 generators for the Lie algebra of skew symmetric 4×4 matrices, written in 3+1 partitioned form, and (following convention) made Hermitian

$$\mathrm{M}_k = i \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{e}_k \times \end{bmatrix} \qquad \mathrm{N}_\ell = i \begin{bmatrix} 0 & -\mathbf{e}_\ell^{\mathrm{T}} \\ \mathbf{e}_\ell & 0_{3\times 3} \end{bmatrix} \qquad k, \ell = 1, 2, 3$$

where column vectors $\mathbf{e}_\ell$ are the standard orthonormal basis vectors in $\mathbb{R}^3$ and $\mathrm{v}\times$ denotes the 3×3 skew-symmetric matrix inducing the cross product with a vector v. We have the following commutation relations:

$$[\mathrm{M}_k, \mathrm{M}_\ell] = i\epsilon_{k\ell j}\mathrm{M}_j \qquad [\mathrm{M}_k, \mathrm{N}_\ell] = i\epsilon_{k\ell j}\mathrm{N}_j \qquad [\mathrm{N}_k, \mathrm{N}_\ell] = i\epsilon_{k\ell j}\mathrm{M}_j \tag{9}$$

Now define an alternative basis

$$\mathrm{K}_\ell = \frac{1}{2}(\mathrm{M}_\ell + \mathrm{N}_\ell) \qquad \mathrm{L}_\ell = \frac{1}{2}(\mathrm{M}_\ell - \mathrm{N}_\ell)$$

In this basis the 6-dimensional Lie algebra $\mathfrak{so}(4)$ splits into two 3-dimensional commuting $\mathfrak{so}(3)$ subalgebras (or equivalently two $\mathfrak{su}(2)$ subalgebras)

$$[\mathrm{K}_k, \mathrm{K}_\ell] = i\epsilon_{k\ell j}\mathrm{K}_j \qquad [\mathrm{K}_k, \mathrm{L}_\ell] = 0 \qquad [\mathrm{L}_k, \mathrm{L}_\ell] = i\epsilon_{k\ell j}\mathrm{L}_j$$

A similar splitting occurs in the 6-dimensional Lie algebra of the Lorentz group, and can be used to classify all irreducible representations.

Recall that irreducible representations of SU(2) are of dimension $2\ell + 1$ with "weights" $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. The splitting of $\mathfrak{so}(4)$ results in irreducible representations of the direct product $\mathrm{SU}(2) \times \mathrm{SU}(2)$ with algebras which are *tensor products* of pairs of $\mathfrak{su}(2)$ represenstions, given by their respective weights (k, ℓ) and having dimension $(2k + 1) \cdot (2\ell + 1)$.

<u>RESULTS</u>:

1. the Lie algebra of SO(4) has generators $(\mathrm{K}_1, \mathrm{K}_2, \mathrm{K}_3)$ and $(\mathrm{L}_1, \mathrm{L}_2, \mathrm{L}_3)$ with commutation relations

$$[\mathrm{K}_k, \mathrm{K}_\ell] = i\epsilon_{k\ell j}\mathrm{K}_j \qquad [\mathrm{K}_k, \mathrm{L}_\ell] = 0 \qquad [\mathrm{L}_k, \mathrm{L}_\ell] = i\epsilon_{k\ell j}\mathrm{L}_j$$

2. Among its other irreducible representations, SO(4) has irreducible representations of dimension

$$n^2 = (2\ell + 1)^2 = 1, 4, 9, 16, \ldots$$

   for $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$

<u>Remark: $\mathrm{SU}(2) \times \mathrm{SU}(2)$ is the double covering of SO(4)</u>

Given $\mathbf{x} = (x_0, x_1, x_2, x_3) = (x_0, \vec{\mathbf{x}}) \in \mathbb{R}^4$, define the 2×2 complex matrix matrix

$$\mathrm{M}(\mathbf{x}) = x_0 \mathrm{I}_{2\times 2} + i\vec{\mathbf{x}} \cdot \vec{\boldsymbol{\sigma}} = \begin{bmatrix} x_0 + ix_3 & ix_1 + x_2 \\ ix_1 - x_2 & x_0 - ix_3 \end{bmatrix}$$

Then

$$\det \mathrm{M}(\mathbf{x}) = |\mathbf{x}|^2 = x_0^2 + x_1^2 + x_2^2 + x_3^2$$

and for any pair of 2×2 unitary matrices $(\mathrm{U}_1, \mathrm{U}_2) \in \mathrm{SU}(2) \times \mathrm{SU}(2)$

$$\mathrm{M}(\mathbf{x}) \to \mathrm{M}(\mathbf{x}') = \mathrm{U}_1 \mathrm{M}(\mathbf{x}) \mathrm{U}_2^\dagger$$

induces a rotation $\mathrm{R} \in \mathrm{SO}(4)$, since $\det \mathrm{M}(\mathbf{x}) = \det \mathrm{M}(\mathbf{x}')$. Since $(\mathrm{U}_1, \mathrm{U}_2)$ and $(-\mathrm{U}_1, -\mathrm{U}_2)$ induce the same rotation, the correspondence

$$\mathrm{SU}(2) \times \mathrm{SU}(2) \to \mathrm{SO}(4)$$

is a double covering map.