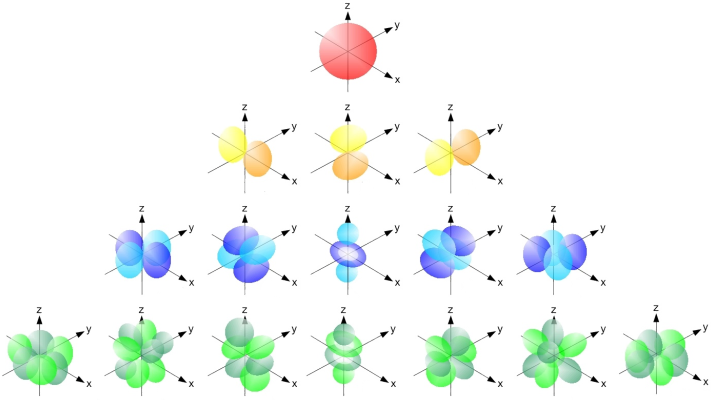
Hidden Symmetries of the Hydrogen Atom



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Classical Mechanics

A particle of mass m moving in a potential $V\colon \mathbb{R}^n \to \mathbb{R}$ feels a force

$$\vec{F} = -\vec{\nabla} V$$

and obeys Newton's law

$$\vec{F} = m\vec{a}$$

so its path $\vec{q}\colon \mathbb{R} \to \mathbb{R}^n$ obeys

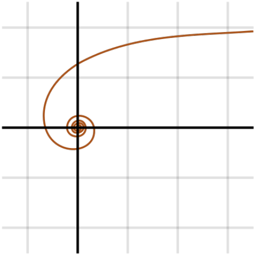
$$m\frac{d^2}{dt^2}\,\vec{q}(t) = -\vec{\nabla} V(\vec{q}(t))$$

A potential like

$$V(\vec{x}) = -\frac{1}{\|\vec{x}\|^p}$$

with $p > 0$ creates a **central force** that pulls the particle towards the origin.

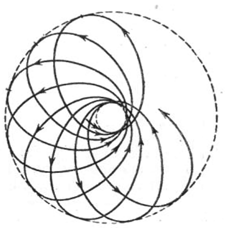
If $p \geq 2$ the particle can easily spiral in to the origin!



If $p < 2$ the particle only hits the origin for initial positions and velocities in a set of measure zero. Otherwise it either:

- Approaches ∞ as $t \to \pm\infty$ (an **unbound** orbit)
- Stays in a compact subset of $\mathbb{R}^n - \{\vec{0}\}$ (a **bound** orbit).

For most choices of p, the bound orbits are typically *not* periodic:



Bertrand's Theorem. If $V\colon \mathbb{R}^n \to \mathbb{R}$ is a spherically symmetric potential all of whose bound orbits are periodic, then either:

$$V(\vec{x}) = k\|\vec{x}\|^2$$

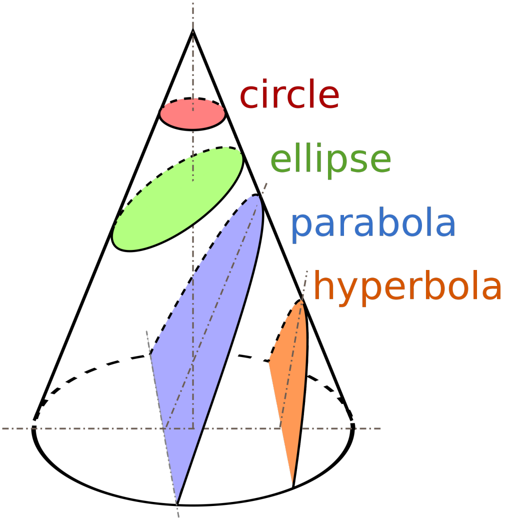
or

$$V(\vec{x}) = -\frac{k}{\|\vec{x}\|}$$

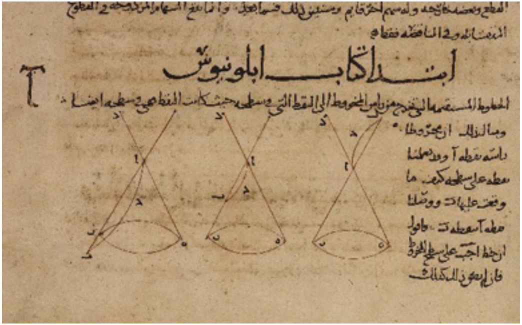
for some $k \geq 0$.

The first case is the **harmonic oscillator.** The second case is the **Kepler problem**: the motion of a particle in the gravitational field of a fixed mass. These are the two most famous exactly solvable problems in classical mechanics.

The Kepler problem has solutions where the particle traces out a conic section:



Amazingly, the theory of conic sections was developed by Apollonius around 200 BC, developed further by the Arabs around 1000 AD...



... and was waiting for Kepler and then Newton, who showed conic sections were the solutions to his differential equation for planets and comets moving around the Sun!

For a particle in any potential, **energy** is conserved:

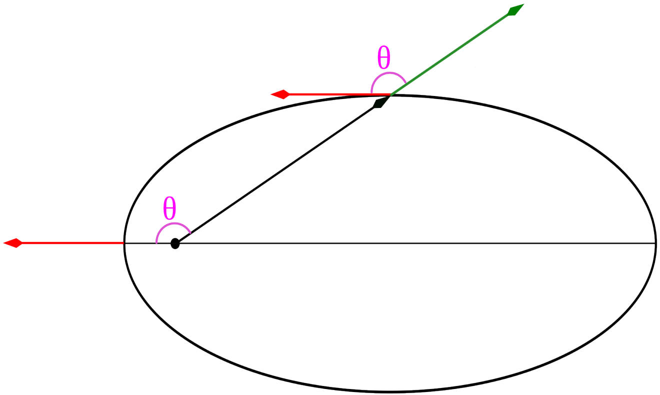
$$E = \frac{1}{2} m \|\dot{\vec{q}}\|^2 + V(\vec{q})$$

For a particle in a central force, **angular momentum** is also conserved. In 3 dimensions it is

$$\vec{J} = m \, \vec{q} \times \dot{\vec{q}}$$

These 4 conserved quantities come from time translation symmetry and rotation symmetry, via Noether's theorem.

But the Kepler problem also has 3 more conserved quantities, the components of the **Laplace–Runge–Lenz vector**! For a bound orbit, this vector always points in the direction of the ellipse's major axis:



The formula for the Laplace–Runge–Lenz vector is unpleasant:

$$\vec{A} = m\dot{\vec{q}} \times \vec{J} - mk\frac{\vec{q}}{\|\vec{q}\|}$$

But it has wonderful properties!

You can use the conservation of $\vec{J}$ and $\vec{A}$ to quickly solve the Kepler problem and prove the solutions are conic sections.

But what is the *meaning* of the Laplace–Runge–Lenz vector?

Noether's theorem relates symmetries to conserved quantities.

The rotation invariance of the 3d Kepler problem gives 3 conserved quantities — the components of angular momentum — because the rotation group $\mathrm{SO}(3)$ is a 3-dimensional Lie group.

But in fact a larger group, $\mathrm{SO}(4)$, acts on the space of bound orbits of the 3d Kepler problem. This is a 6-dimensional Lie group.

These 'hidden symmetries' give 3 more conserved quantities: the components of the Laplace–Runge–Lenz vector!

To understand these hidden symmetries, go down a dimension and look at the 2d Kepler problem.

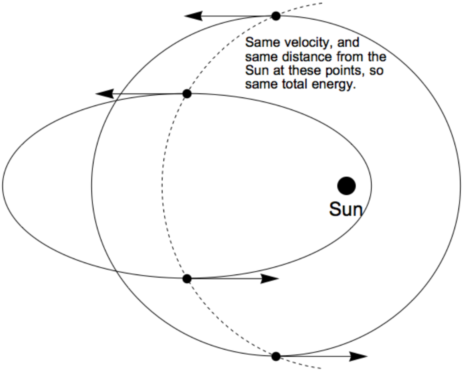
We can rotate any solution and get a new solution with the same energy: this gives an action of $\mathrm{SO}(2)$. How can we extend this to an action of $\mathrm{SO}(3)$?

For a great explanation, see:

- Greg Egan, The ellipse and the atom.

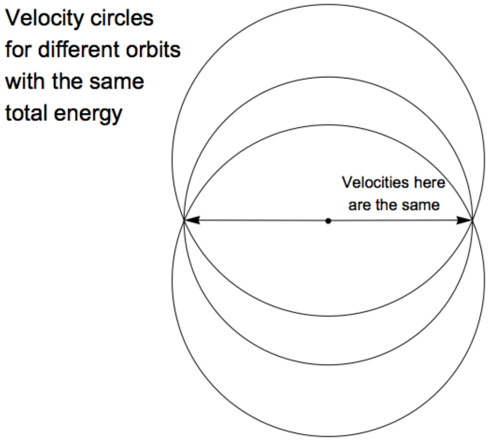
I'll borrow some pictures and ideas from there!

We can transform any elliptical orbit to others with the same energy by taking the particle at either point where it's travelling parallel to the axis of the ellipse, and swinging it along a circular arc centered on the Sun, while keeping its velocity the same:

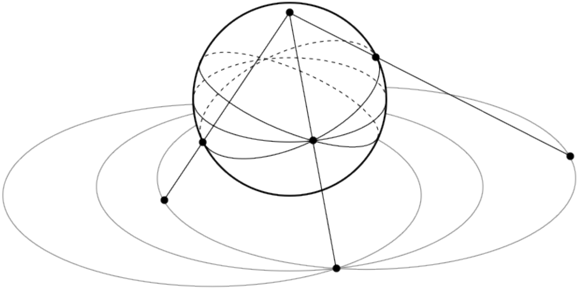


These are some of the hidden symmetries.

Less obviously, the velocity vector of any elliptical orbit traces out a *circle!* The orbits just discussed give circles that meet at two points:

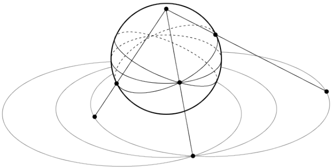


Such circles are obtained by stereographically projection from great circles on a 2-sphere of suitable radius!



The hidden symmetries are rotations of this 2-sphere. They form the group $SO(3)$.

In the end, we get $\mathrm{SO}(3)$ acting on the space of bound orbits of a fixed energy!



This space is isomorphic to the **unit tangent bundle** of S^2:

$$\{(x, v) \in TS^2 : \ x \in S^2, \ v \in T_x S^2, \ \|v\| = 1\}$$

or equivalently the unit cotangent bundle. The action of $\mathrm{SO}(3)$ is the natural one. The space of *all* bound orbits is isomorphic to the **punctured cotangent bundle**

$$T^+ S^2 = \{(x, p) \in T^* S^2 : \ x \in S^2, \ p \in T_x^* S^2, \ p \neq 0\}$$

All this generalizes easily to the 3d Kepler problem!

- The velocity vectors of all bound orbits of fixed energy trace out circles in $\mathbb{R}^3$ that are stereographic projections of great circles in S^3.
- The space of all bound orbits is isomorphic to the punctured cotangent bundle T^+S^3.
- $\mathrm{SO}(4)$ acts on this space in a natural way.

The Hydrogen Atom

Even more wonderfully, the Kepler problem is also what we need to understand the hydrogen atom. The electron moves in a potential

$$V(\vec{x}) = -\frac{k}{\|\vec{x}\|}$$

attracted by the much heavier proton, just as a planet is attracted by the heavier Sun! But to understand the hydrogen atom we need the *quantum* version of the Kepler problem.

This was figured out by Bohr, Sommerfeld, de Broglie, Schrödinger, Heisenberg and many others. Pauli and Fock used the Laplace–Runge–Lenz vector!

Quantum Mechanics

A particle of mass m moving in a potential $V\colon \mathbb{R}^n \to \mathbb{R}$ has a wavefunction $\psi\colon \mathbb{R} \times \mathbb{R}^n \to \mathbb{C}$ obeying **Schrödinger's equation**

$$i\hbar \frac{\partial}{\partial t}\psi(t, \vec{x}) = -\frac{\hbar^2}{2m}\nabla^2\psi(t, x) + V(\vec{x})\psi(t, \vec{x})$$

where $\hbar$ is Planck's constant.

More abstractly, and choosing units where $\hbar = 2m = 1$, Schrödinger's equation is

$$\frac{\partial \psi}{\partial t} = -iH\psi$$

where the **Hamiltonian** H is

$$H = -\nabla^2 + V$$

If the operator H is self-adjoint on $L^2(\mathbb{R}^n)$, we can solve Schrödinger's equation by

$$\psi(t) = e^{-itH}\psi(0)$$

where $\psi(t) \in L^2(\mathbb{R}^3)$ is the wavefunction at time t.

For the 3d Kepler problem, choosing units where $k = 1$,

$$H = -\nabla^2 - \frac{1}{\|\vec{x}\|}$$

is indeed a self-adjoint operator on $L^2(\mathbb{R}^3)$, so this method works. But it's only practical if we know the eigenvectors of H.

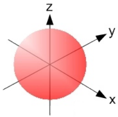
The **spectrum** of a self-adjoint operator H is the set of numbers λ such that $H - \lambda I$ does not have a bounded inverse. For the 3d Kepler problem, the spectrum is

$$\left\{-\frac{1}{4n^2}\right\}_{n=1}^{\infty} \cup [0, \infty)$$

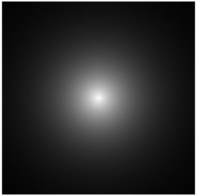
The negative numbers in the spectrum are eigenvalues of H; the eigenvectors are **bound states**, the quantum analogue of bound orbits.

All nonnegative numbers are in the spectrum; these correspond to **scattering states**, the quantum analogue of unbound orbits. We shall not discuss these, even though they're interesting!

The space of eigenvectors ψ with $H\psi = -\frac{1}{4n^2}\psi$ is 1-dimensional when $n = 1$. Here's one:

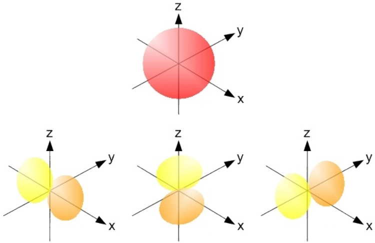


or more accurately:



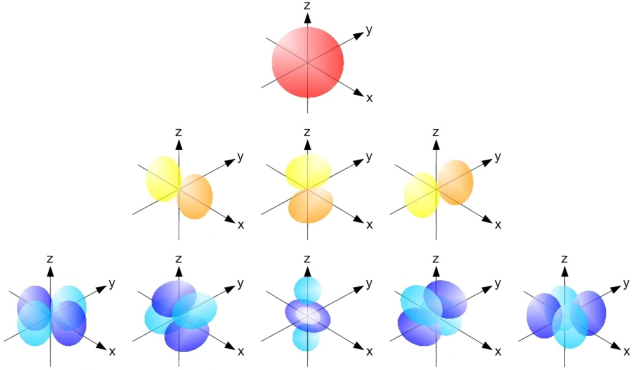
This space is the 1-dimensional trivial representation of $\mathrm{SO}(3)$.

The space of eigenvectors ψ with $H\psi = -\frac{1}{4n^2}\psi$ is 4-dimensional when $n = 2$.



It's the direct sum of the 1d and 3d irreducible representations of $\mathrm{SO}(3)$.

The space of eigenvectors ψ with $H\psi = -\frac{1}{4n^2}\psi$ is 9-dimensional when $n = 3$.



It's the direct sum of the 1d, 3d and 5d irreducible representations of $\mathrm{SO}(3)$. And so on....

The space

$$\mathcal{H}_n = \left\{\psi \in L^2(\mathbb{R}^n) : H\psi = -\frac{1}{4n^2}\psi\right\}$$

has dimension n^2. It's a unitary representation of $\mathrm{SO}(3)$, and it's a direct sum of irreducible representations of dimensions $1, 3, 5, \ldots, 2n-1$.

But in fact $\mathcal{H}_n$ is a representation of $\mathrm{SO}(4)$! In quantum mechanics, the components of angular momentum and the Laplace–Runge–Lenz vectors become self-adjoint operators on $L^2(\mathbb{R}^n)$, and these generate a unitary representation of $\mathrm{SO}(4)$ on this space, with $\mathcal{H}_n$ as an invariant subspace.

Indeed, the space of bound states of the 3d Kepler problem is isomorphic to $L^2(S^3)$:

$$L^2(S^3) \cong \bigoplus_{n=1}^{\infty} \mathcal{H}_n$$

and the action of $\mathrm{SO}(4)$ on the sphere S^3 gives its representation on the space of bound states! Each summand $\mathcal{H}_n$ is an **irrep** of $\mathrm{SO}(4)$: an irreducible representation.

This becomes more beautiful using the Peter–Weyl theorem.

Peter–Weyl Theorem. Suppose G is a compact topological group equipped with its **Haar measure**, the unique translation-invariant Borel measure μ with $\mu(G) = 1$. Then

$$L^2(G) \cong \bigoplus_{\rho} \rho \otimes \rho^*$$

as representations of $G \times G$. Here $G \times G$ acts on G by left and right translations, and ρ runs over representatives of all isomorphism classes of continuous irreps of G.

All the continuous irreps ρ of G are finite-dimensional. Each space $\rho \otimes \rho^*$ is an irrep of $G \times G$.

We can think of S^3 as $\mathrm{SU}(2)$. Then $\mathrm{SU}(2) \times \mathrm{SU}(2)$ acts as left and right translations of $\mathrm{SU}(2)$. We get all rotations of S^3 this way, giving a double cover

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

There's a continuous irrep of $\mathrm{SU}(2)$ on $S^n(\mathbb{C}^2)$, the space of homogeneous degree-n polynomials in 2 variables:

$$S^n(\mathbb{C}^2) \cong \left\{ a_0 x^n + a_1 x^{n-1} y + \cdots + a_{n-1} x y^{n-1} + a_n y^n : a_i \in \mathbb{C} \right\}$$

This representation has dimension $n+1$. Every continuous irrep of $\mathrm{SU}(2)$ is isomorphic to one of these! So, they're all self-dual.

Putting these facts together, we get

$$L^2(S^3) \cong \bigoplus_{n=0}^{\infty} S^n(\mathbb{C}^2) \otimes S^n(\mathbb{C}^2)$$

as representations of $\mathrm{SU}(2) \times \mathrm{SU}(2)$, and indeed $\mathrm{SO}(4)$.

In fact this is just another view of our decomposition

$$L^2(S^3) \cong \bigoplus_{n=1}^{\infty} \mathcal{H}_n$$

where

$$\mathcal{H}_n = \left\{ \psi \in L^2(\mathbb{R}^n) : H\psi = -\frac{1}{4n^2}\psi \right\}$$

So

$$\mathcal{H}_n \cong S^{n-1}(\mathbb{C}^2) \otimes S^{n-1}(\mathbb{C}^2)$$

and this is the deep reason why

$$\dim(\mathcal{H}_n) = n^2$$

There is *much* more to say, but go here for more:

- John Baez, Mysteries of the gravitational 2-body problem.