

Second Quantization of the Kepler Problem

the atom,



the solar system,



and the universe



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Integrable Systems and Mathematical Physics Seminar

September 22, 2026

The classical particle moving in an elliptical orbit in an inverse square force $\cong$
the classical relativistic free massless spin-0 particle in $\mathbb{R} \times S^3$

⇓ quantization

The nonrelativistic hydrogen atom with spin-0 electron $\cong$
the quantum relativistic free massless spin-0 particle in $\mathbb{R} \times S^3$

⇓ including spin

The nonrelativistic hydrogen atom with spin- $\frac{1}{2}$ electron $\cong$
the quantum relativistic free massless spin- $\frac{1}{2}$ particle in $\mathbb{R} \times S^3$

⇓ second quantization

The atom with many noninteracting spin- $\frac{1}{2}$ electrons $\cong$
the massless spin- $\frac{1}{2}$ relativistic free quantum field in $\mathbb{R} \times S^3$

The classical Kepler problem

If we work in units where the inverse square force law says

$$\ddot{\mathbf{q}} = -\frac{\mathbf{q}}{q^3}$$

and define momentum by $\mathbf{p} = \dot{\mathbf{q}}$, then not only are energy

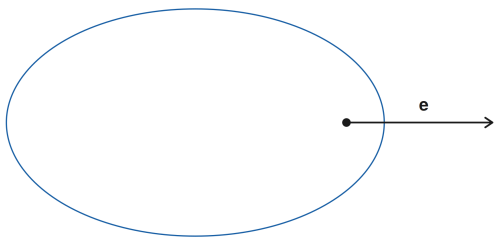
$$E = \frac{1}{2}p^2 - \frac{1}{q}$$

and angular momentum

$$\mathbf{L} = \mathbf{q} \times \mathbf{p}$$

conserved, but also another vector:

$$\mathbf{e} = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{q}}{q}$$



$$\mathbf{e} = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{q}}{q}$$

This vector always points in the direction of the orbit's perihelion, and its magnitude e equals the eccentricity of the orbit.

$$\mathbf{e} = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{q}}{q}$$

This extra conserved quantity was named the 'Runge–Lenz vector' after Lenz used it in 1924 to study the hydrogen atom, citing Runge's popular textbook from five years earlier.

But Runge never claimed any originality: he attributed this vector to Gibbs. Now some call it the 'Laplace–Runge–Lenz vector', honoring Laplace's discussion of it in 1799.

But in fact this vector goes back at least to Jakob Hermann, who wrote about it in 1710, triggering further work by Johann Bernoulli in the same year.

I will call $\mathbf{e}$ the **eccentricity vector**.

Which extra symmetries give conservation of the eccentricity vector? Starting from $\{q_j, p_k\} = \delta_{jk}$, some calculations give

$$\begin{aligned}\{L_j, L_k\} &= \epsilon_{jkl} L_l \\ \{e_j, L_k\} &= \epsilon_{jkl} e_l \\ \{e_j, e_k\} &= -2E \epsilon_{jkl} L_l\end{aligned}$$

and of course

$$\{E, L_j\} = \{E, e_j\} = 0$$

since $\mathbf{L}$ and $\mathbf{e}$ are conserved. The factor of $-2E$ above is annoying, but on the region of phase space where $E < 0$ — that is, the space of bound states — we can define a vector

$$\mathbf{M} = \frac{\mathbf{e}}{\sqrt{-2E}}$$

and obtain

$$\begin{aligned}\{L_j, L_k\} &= \epsilon_{jkl} L_l \\ \{L_j, M_k\} &= \epsilon_{jkl} M_l \\ \{M_j, M_k\} &= \epsilon_{jkl} M_l\end{aligned}$$

This gives a Lie algebra isomorphic to $\mathfrak{so}(3) \oplus \mathfrak{so}(3)$, as becomes clear if we set

$$\mathbf{A} = \frac{1}{2}(\mathbf{L} + \mathbf{M}), \quad \mathbf{B} = \frac{1}{2}(\mathbf{L} - \mathbf{M})$$

and check that

$$\begin{aligned}\{A_j, A_k\} &= \epsilon_{jkl} A_l \\ \{B_j, B_k\} &= \epsilon_{jkl} B_l \\ \{A_j, B_k\} &= 0\end{aligned}$$

But $\mathfrak{so}(3) \oplus \mathfrak{so}(3) \cong \mathfrak{so}(4)$, so conservation of the eccentricity vector must come from a hidden $\mathfrak{so}(4)$ symmetry.

And indeed, the group $SO(4)$ acts on the bound states of the Kepler problem in a way that commutes with time evolution! We can understand this geometrically.

In 1847 Hamilton discovered another remarkable feature of the inverse square force law: the momentum $\mathbf{p}$ moves in a circle!

Solving

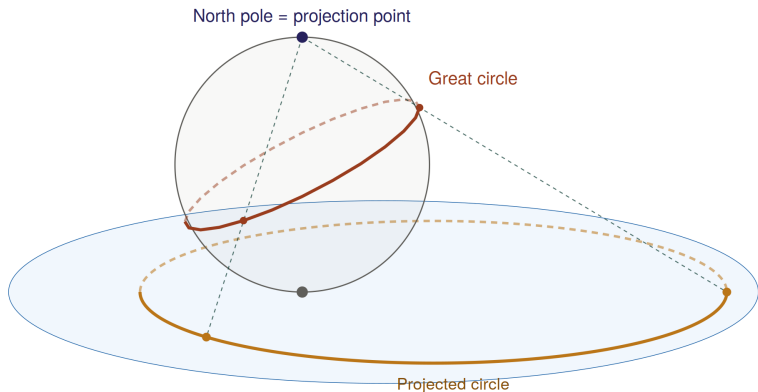
$$\mathbf{e} = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{q}}{q}$$

for $\mathbf{q}/q$, taking the dot product of this with itself, which is 1, and doing some further manipulations, we can show

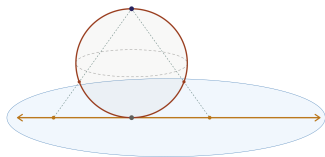
$$\left(\mathbf{p} - \frac{\mathbf{L} \times \mathbf{e}}{L^2} \right)^2 = \frac{1}{L^2}.$$

Thus, $\mathbf{p}$ moves along a circle centered at the point $(\mathbf{L} \times \mathbf{e})/L^2$.

Hamilton's momentum circles are not arbitrary circles in $\mathbb{R}^3$. Using the inverse of stereographic projection, we can map $\mathbb{R}^3$ to the unit 3-sphere. This sends Hamilton's circles in $\mathbb{R}^3$ to great circles in S^3 .



Hamilton's construction gives all the great circles in S^3 except those that go through the north and south poles of S^3 .



These missing great circles correspond to periodic orbits of infinite eccentricity where a particle starts with momentum zero, falls straight to the origin, then bounces back the way it came!

We can embed the phase space of bound states of the Kepler problem, as a symplectic manifold, into T^*S^3 in such a way that these additional orbits become legitimate trajectories in T^*S^3 .

Now every great circle on S^3 corresponds to a periodic orbit of a particle in the attractive inverse square force.

As time passes, the momentum moves along a great circle in S^3 .
How is the dynamics related to geodesic motion on the 3-sphere?

We can understand this as follows. If E is the Hamiltonian for the Kepler problem — the particle in the attractive inverse square force — a calculation shows

$$-\frac{1}{E} = L^2 + M^2$$

Using the fact that $\mathbf{L} \cdot \mathbf{M} = 0$ and the definitions

$$\mathbf{A} = \frac{1}{2}(\mathbf{L} + \mathbf{M}), \quad \mathbf{B} = \frac{1}{2}(\mathbf{L} - \mathbf{M})$$

an easy calculation gives

$$-\frac{1}{E} = 8A^2 = 8B^2$$

In the 3-sphere picture, the observables A_j become functions on T^*S^3 . These functions are just the components of momentum for a particle on S^3 , defined using a standard basis of right-invariant vector fields on $S^3 \cong \text{SU}(2)$.

Similarly, the observables B_j are the components of momentum using a standard basis of left-invariant vector fields. Since nonrelativistic kinetic energy $\propto \text{momentum}^2$,

$$K = 8A^2 = 8B^2$$

is the Hamiltonian for a nonrelativistic free particle on S^3 with an appropriately chosen mass.

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is the Hamiltonian for a nonrelativistic free particle on S^3 with an appropriately chosen mass. This means

$$K = 8A^2 = 8B^2 = -\frac{1}{E}$$

where E is the energy of the particle in the Kepler problem!

A nonrelativistic free particle on S^3 moves around a great circle at constant speed. Since the Kepler Hamiltonian E is $-1/K$, particles governed by *this* Hamiltonian move along the same trajectories — but typically not at constant speed.

Both K and the Kepler Hamiltonian $E = -1/K$ are well-defined smooth functions on the symplectic manifold that Souriau dubbed the **Kepler manifold**:

$$T^+S^3 = \{(x, p) : x \in S^3, p \in T_x S^3, p \neq 0\}.$$

We can also think of

$$T^+S^3 = \{(x, p) : x \in S^3, p \in T_x S^3, p \neq 0\}.$$

as the space of light rays in the **Einstein universe**: the manifold $\mathbb{R} \times S^3$ with Lorentzian metric $dt^2 - ds^2$, where ds^2 is the usual metric on the unit 3-sphere. Here a **light ray** is a null geodesic equipped with a choice of covariantly constant tangent vector field, its '4-velocity'.

To describe a light ray using a point in T^+S^3 , let $x \in S^3$ be the light ray's position at time zero, while the null cotangent vector $p + \|p\|dt$ describes the light ray's energy-momentum at time zero.

In this way T^+S^3 serves as a phase space for a classical free *massless* relativistic particle in the Einstein universe. The Hamiltonian for such a particle is $\sqrt{K}$.

Summary so far

On the phase space T^*S^3 let

$$K = 8A^2 = 8B^2 \propto \text{momentum}^2$$

We have the following classical Hamiltonians:

- ▶ massive nonrelativistic particle in S^3 : K
- ▶ massless relativistic particle in $\mathbb{R} \times S^3$: $\sqrt{K}$
- ▶ Kepler problem: $E = -1/K$.

Quantizing the Kepler problem

We can quantize the bound states of a particle in the inverse square force using the Hilbert space $L^2(S^3)$. A point on S^3 is a momentum eigenstate.

Since $S^3 \cong \text{SU}(2)$, there is a unitary representation R of $\text{SU}(2) \times \text{SU}(2)$ on $L^2(S^3)$ given by left and right translations.

$$(R(g, g')\psi)(h) = \psi(g^{-1}h g')$$

If we call the self-adjoint generators of these left and right translations A_k and B_k ($k = 1, 2, 3$), we have

$$\begin{aligned}[A_j, A_k] &= i\epsilon_{jkl}A_l \\ [B_j, B_k] &= i\epsilon_{jkl}B_l \\ [A_j, B_k] &= 0\end{aligned}$$

As a representation of $SU(2) \times SU(2)$, we have

$$L^2(S^3) \cong \bigoplus_j V_j \otimes V_j$$

where $j = 0, \frac{1}{2}, 1, \dots$ and V_j is the spin- j representation of $SU(2)$.

The operators A_k act on the first copy of V_j as the usual angular momentum operators on the spin- j representation, while the operators B_k act on the second copy.

Thus, the operator $A^2 = B^2$ has eigenvalue $j(j+1)$ on $V_j \otimes V_j$, and the multiplicity of this eigenvalue is $(2j+1)^2$.

This matches what we see in the hydrogen atom: not counting spin, there are n^2 eigenstates in the n th energy level.

The Hamiltonian for bound states of the *quantum* particle in the inverse square force is

$$H_0 = -\frac{1}{8(A^2 + \frac{1}{4})} = -\frac{1}{8(B^2 + \frac{1}{4})}$$

This differs from the classical Hamiltonian by the extra $+\frac{1}{4}$, which can be explained using the Duflo isomorphism. With this correction, the eigenvalues match the energy levels of the bound states of hydrogen — treated nonrelativistically, and ignoring the electron's spin.

There's a nice geometrical meaning: $A^2 = B^2$ is proportional to the positive definite Laplacian on S^3 :

$$A^2 = B^2 = \frac{1}{4}\Delta$$

Introducing spin

Now let's introduce spin, but still for bound states of the *nonrelativistic* hydrogen atom. This just doubles the Hilbert space to $L^2(S^3) \otimes \mathbb{C}^2$. The Hamiltonian is now

$$H = H_0 \otimes 1$$

where H_0 is the Hamiltonian we just saw in the spin-zero case.

If we trivialize the spinor bundle on S^3 using the right translation action of $SU(2)$, we can think of $\psi \in L^2(S^3) \otimes \mathbb{C}^2$ as a spinor field on S^3 . Then we can show

$$H = -\frac{1}{2(\not{D} - \frac{1}{2})^2}$$

where $\not{D}$ is the Dirac operator on the 3-sphere.

Chiral massless spin-1/2 particles on $\mathbb{R} \times S^3$ are described by fields

$$\psi: \mathbb{R} \times S^3 \rightarrow \mathbb{C}^2$$

The **left-handed Weyl equation** is

$$\frac{\partial \psi}{\partial t} = -i \not{\partial} \psi$$

where $\not{\partial}$ is the Dirac operator on S^3 . We can use $L^2(S^3) \otimes \mathbb{C}^2$ as a Hilbert space of initial data; then $\not{\partial}$ is an unbounded self-adjoint operator that we can use as the Hamiltonian.

$SU(2) \times SU(2)$ acts on this Hilbert space with generators A_k and $B_k + S_k$, S_k being spin angular momentum. $\not{\partial}$ commutes with this group action.

But there's a problem: the Dirac operator $\not{D}$ has a spectrum that's unbounded below! To fix this in one-particle relativistic quantum mechanics we can just change the complex structure on $L^2(S^3) \otimes \mathbb{C}^2$ to

$$j = i \frac{\not{D}}{|\not{D}|}$$

and use the Hamiltonian $|\not{D}|$, which has only positive eigenvalues. Notice $i\not{D} = j|\not{D}|$, so the left-handed Weyl equation

$$\frac{\partial \psi}{\partial t} = -i\not{D}\psi$$

is equivalent to

$$\frac{\partial \psi}{\partial t} = -j|\not{D}|\psi$$

But now the Hamiltonian is positive! Call $L^2(S^3) \otimes \mathbb{C}^2$ with this new complex structure **H**.

In fact there's a unitary equivalence

$$F: L^2(S^3) \otimes \mathbb{C}^2 \xrightarrow{\sim} \mathbf{H}$$

that commutes with the representation of $SU(2) \times SU(2)$ and the Dirac operator on each space!

This lets us make both the Hamiltonian for the hydrogen atom with electron spin

$$H = -\frac{1}{2(\not{\partial} - \frac{1}{2})^2}$$

and the Hamiltonian for the left-handed massless spin-1/2 particle

$$|\not{\partial}|$$

into operators on the *same* space. The second operator is a function of the first.

Second quantization

Define a fermionic Fock space by forming the exterior algebra

$$\Lambda(L^2(S^3) \otimes \mathbb{C}^2) \cong \Lambda \mathbf{H}$$

and taking its Hilbert space completion $\mathbf{K}$. States in $\mathbf{K}$ describe collections of fermions, like $\psi_1 \wedge \cdots \wedge \psi_N$ where $\psi_i \in \mathbf{H}$.

On the one hand, $\mathbf{K}$ is the Hilbert space for *noninteracting collections of electrons orbiting a nucleus*: a very simple toy model of an atom.

On the other hand, it's the Hilbert space for *noninteracting collections of left-handed massless spin-1/2 fermions in $\mathbb{R} \times S^3$* : a massless spin-1/2 free quantum field.

Any 1-particle Hamiltonian A on $\mathbf{H}$ gives a multiparticle Hamiltonian $d\Lambda(A)$ on $\mathbf{K}$. For example

$$d\Lambda(A)(\psi_1 \wedge \psi_2 \wedge \psi_3) =$$

$$A\psi_1 \wedge \psi_2 \wedge \psi_3 + \psi_1 \wedge A\psi_2 \wedge \psi_3 + \psi_1 \wedge \psi_2 \wedge A\psi_3$$

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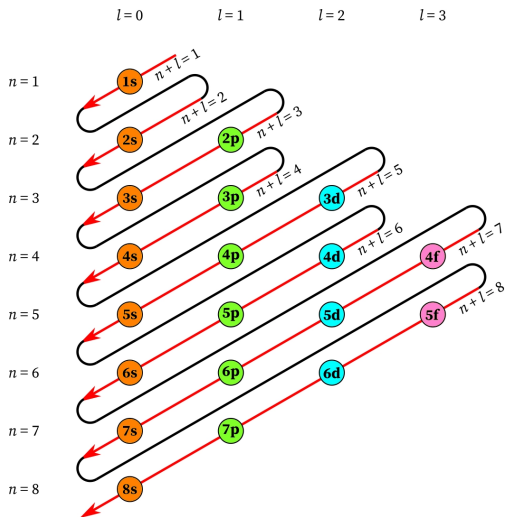
If we start with the Hamiltonian H for the hydrogen atom, and for each N take the lowest-energy N -electron state for the Hamiltonian $d\Lambda(H)$, we don't get the periodic table. Instead, we fill in states of

$$\mathbf{H} \cong L^2(S^3) \otimes \mathbb{C}^2 \cong \bigoplus_j V_j \otimes V_j \otimes \mathbb{C}^2$$

according to increasing values of $j = 0, \frac{1}{2}, 1, \dots$, with $2n^2 = 2(2j+1)^2$ electrons in each "shell", all with the same energy.

In 1936, Madelung argued for these rules:

- ▶ states are filled in order of increasing value of $n + \ell$;
- ▶ states with the same value of $n + \ell$ are filled in order of decreasing ℓ .



We can get the Madelung rules if we take a suitable single-particle Hamiltonian H_{single} on $\mathbf{H}$, form the multiparticle Hamiltonian $d\Lambda(H_{\text{single}})$ on $\mathbf{K}$, and for each N take the lowest-energy N -electron state for the Hamiltonian $d\Lambda(H_{\text{single}})$.

So, we get a pretty good approximation to the periodic table from a suitable fermionic quantum field theory on $\mathbb{R} \times S^3$!

$n = 1$	1 H Hydrogen	2 He Helium																
$n = 2$	3 Li Lithium	4 Be Beryllium											5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
$n = 3$	11 Na Sodium	12 Mg Magnesium											13 Al Aluminum	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon
$n = 4$	19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
$n = 5$	37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
$n = 6$	55 Cs Cesium	56 Ba Barium	71 Lu Lutetium	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
$n = 7$	87 Fr Francium	88 Ra Radium	103 Lr Lawrencium	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Cn Copernicium	113 Nh Nihonium	114 Fl Flerovium	115 Mc Moscovium	116 Lv Livermorium	117 Ts Tennessine	118 Og Oganesson

■ s subshells: $\ell = 0$

■ d subshells: $\ell = 1$

■ p subshells: $\ell = 2$

■ f subshells: $\ell = 3$

57 La Lanthanum	58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium
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89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium
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