Runge-Lenz method for the energy level of hydrogen atom

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Runge-Lentz (or Laplace-Runge-Lentz) vector

In classical mechanics, the **Runge–Lenz vector** (or simply the **RL vector**) is a vector used chiefly to describe the shape and orientation of the orbit of one astronomical body around another, such as a planet revolving around a star. For two bodies interacting by Newtonian gravity, the LRL vector is a constant of motion, meaning that it is the same no matter where it is calculated on the orbit; equivalently, the LRL vector is said to be *conserved*. More generally, the RL vector is conserved in all problems in which two bodies interact by a central force that varies as the inverse square of the distance between them; such problems are called Kepler problems.

The hydrogen atom is a Kepler problem, since it comprises two charged particles interacting by Coulomb's law of electrostatics, another inverse square central force. The RL vector was essential in the first quantum mechanical derivation of the spectrum of the hydrogen atom, before the development of the Schrödinger equation. However, *this approach is rarely used today*.

http://en.wikipedia.org/wiki/Laplace%E2%80%93Runge%E2%80%93Lenz_vector

Wolfgang Pauli in 1926 used the matrix mechanics of Heisenberg to give the first derivation of the energy levels of hydrogen and their degeneracies. Pauli's derivation is based on the Runge-Lenz vector multiplied by the particle mass. [W. Pauli, Z. Physik 36, 336 (1926).]

1. Kepler's law of planetary motion

The Kepler's laws (I, II, and III) describe the motion of planets around the Sun,

(I) The orbit of a planet is an ellipse with the Sun at one of the two foci.

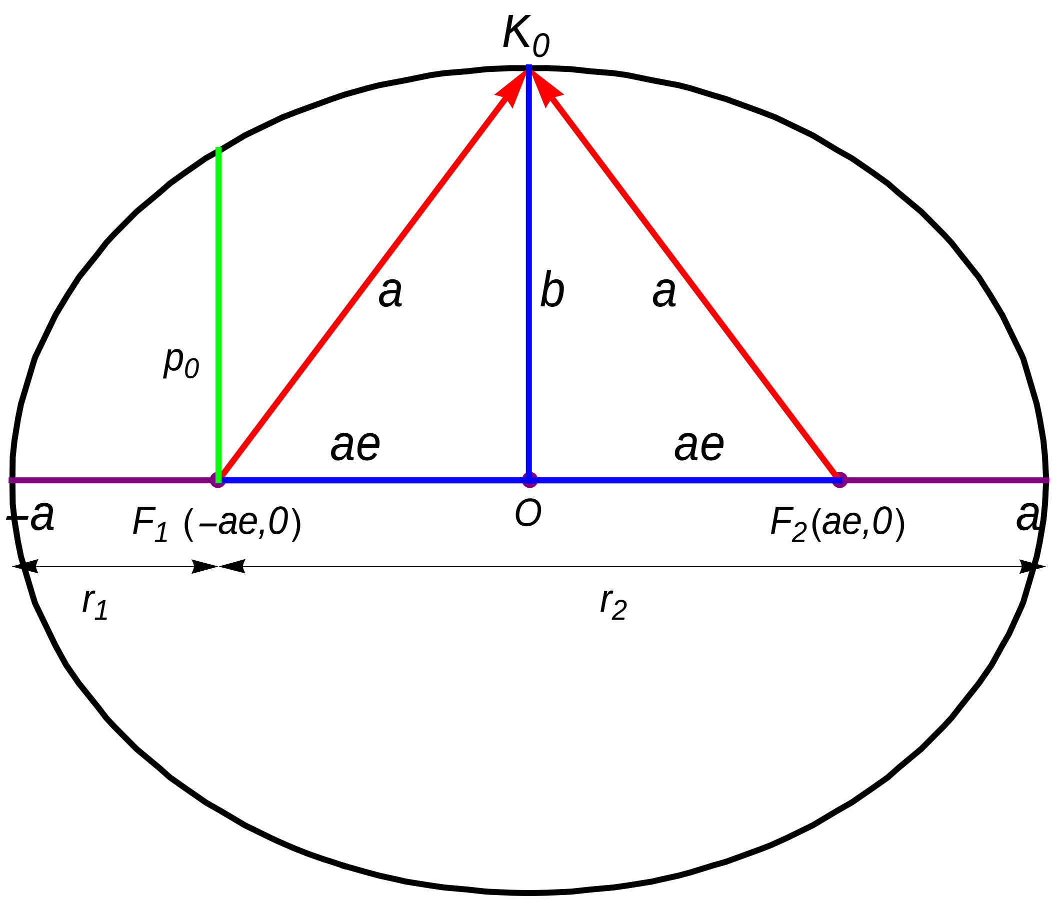
(II) A line segment joining a planet and the Sun sweeps out equal areas during equal interval of time.

(III) The square of the orbital period of a planet is proportional to the cube of the semi-major axis of its orbit.

The Sun is at the one focus of the ellipse (the planet orbit). The ellipse orbit is described by

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1\,.$$

where a is the semi-major axis, b is the semi-minor axis, and e is the eccentricity ($0<e<1$).



(i) The eccentricity *e*

From the definition of ellipsoid, we have

$$\overline{F_1K_0} + \overline{F_2K_0} = 2a$$

When $\overline{F_1K_0} = \overline{F_2K_0}$, we have $\overline{F_1K_0} = \overline{F_2K_0} = a.$ We apply the Pythagorean theorem to the triangle F_1OK_0,

$$a^2 = b^2 + a^2e^2,$$

Then we have the expression for the eccentricity

$$e = \sqrt{1 - \frac{b^2}{a^2}}$$

Note that

$$b = a\sqrt{1-e^2} .$$

(ii) The perihelion and aphelion

The focus is at (ae,0) and (-ae,0). For simplicity, we assume that Sun is located at focus (-ae,0).

The perihelion (r_1) the point nearest the Sun

$$r_1 = a(1-e) ,$$

The aphelion (r_2) the point farthest the Sun

$$r_2 = a(1+e)$$

(iii) Area of the ellipsoid:

The area of the ellipse orbit is given by

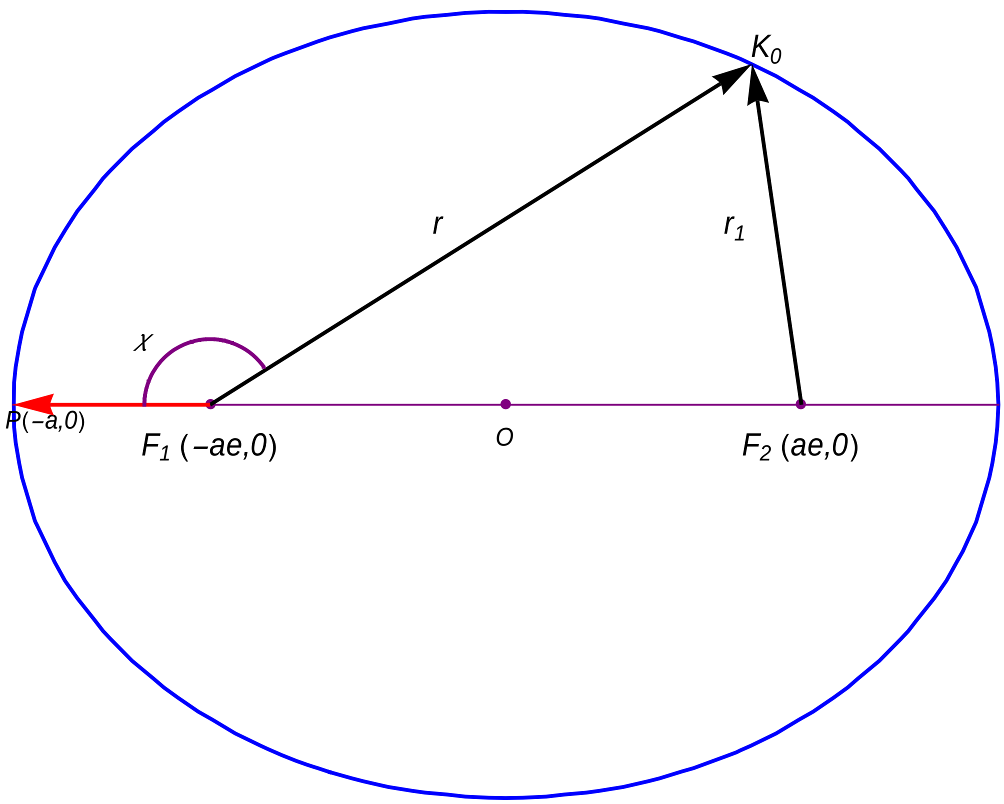
$$A = \pi ab = \pi a^2 \sqrt{1-e^2} .$$

(iv) The mathematical formula the ellipsoid:

Here we show that mathematically, an ellipse can be represented by the formula

$$r = \frac{p_0}{1 + e\cos\chi} ,$$

where p_0 is the semi-latus rectum, and e is the eccentricity of the ellipse, r is the distance from the Sun to the planet, and χ is the angle to the planet's current position K_0 from its closest point P (perihelion), as seen from the Sun at F_1. We use p_0 instead of p since p is typically a linear momentum in physics. We also use χ instead of θ, for convenience.



In the triangle $F_1F_2K_0$ (see the above figure), we have

$$r + r_1 = 2a, \tag{1}$$

from the definition of the ellipse. Using the cosine law, we have

$$r_1^2 = r^2 + 4a^2e^2 - 4aer\cos(\pi - \chi) = r^2 + 4a^2e^2 + 4aer\cos\chi . \tag{2}$$

where χ is the angle between the vector $\overrightarrow{F_1P}$ and $\overrightarrow{F_1K_0}$. From Eqs.(1) and (2), we get

$$(2a - r)^2 = r^2 + 4a^2e^2 + 4aer\cos\chi$$

or

$$4a^2 - 4ar + r^2 = r^2 + 4a^2e^2 + 4aer\cos\chi$$

or

$$r(1 + e\cos\chi) = a(1 - e^2) = p_0$$

or

$$r = \frac{p_0}{1 + e\cos\chi},$$

with

$$p_0 = a(1 - e^2),$$

where (r, χ) are heliocentric polar coordinates for the planet, p_0 is the *semi latus rectum*, and e is the *eccentricity*, which is less than one.

For $\chi = 0$ the planet is at the perihelion at minimum distance:

$$r_1 = \frac{p_0}{1+e} = \frac{a(1-e^2)}{1+e} = a(1-e)\,. \qquad \text{(perihelion)}$$

For $\chi = \frac{\pi}{2}$,

$$r = p_0\,. \qquad \text{(\textit{semi latus rectum})}$$

For $\chi = \pi$, the planet is at the aphelion at maximum distance:

$$r_2 = \frac{p_0}{1-e} = a(1+e)\,. \qquad \text{(aphelion)}$$

Note that

$$\frac{1}{r_1} + \frac{1}{r_2} = \frac{1+e}{p_0} + \frac{1-e}{p_0} = \frac{2}{p_0}\,.$$

The semi-major axis a is the arithmetic mean between r_1 and r_2,

$$a = \frac{r_1 + r_2}{2}\,.$$

The semi-minor axis b is the geometric mean between r_1 and r_2,

$$b = \sqrt{r_1 r_2} = \frac{p_0}{\sqrt{1-e^2}}$$

((**Note**)) The meaning of *semi latus rectum*

The chord through a focus parallel to the conic section directrix of a conic section is called the latus rectum, and half this length is called the semilatus rectum (Coxeter 1969). "Semilatus rectum" is a compound of the Latin *semi*-, meaning half, *latus*, meaning 'side,' and *rectum*, meaning 'straight.'

2. Kepler problem in classical mechanics (hydrogen atom)

The classical Hamiltonian for the Kepler problem is

$$H = \frac{1}{2m}\boldsymbol{p}^2 - \frac{\kappa}{r},$$

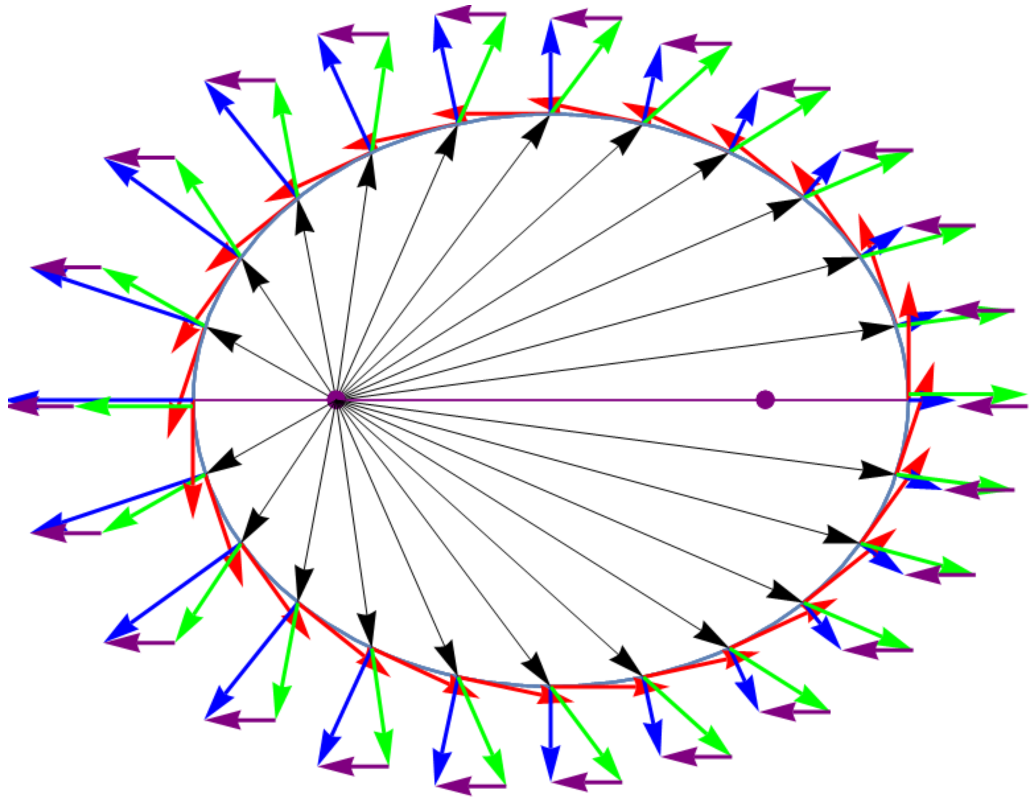
where m is a reduced mass and κ is a positive quantity. For the case of the hydrogen-like atom, we can identify $\kappa = Ze^2$. This system is invariant under the rotation. So the angular momentum is conserved. The classical orbit of the particle is elliptical. The Runge-Lentz vector is defined as

$$\boldsymbol{M} = -\frac{\kappa}{r}\boldsymbol{r} + \frac{1}{m}\boldsymbol{p}\times\boldsymbol{L},$$

or

$$\boldsymbol{A} = m\boldsymbol{M} = -m\kappa\boldsymbol{e}_r + \boldsymbol{p}\times\boldsymbol{L},$$

where $\boldsymbol{L}$ (= $\boldsymbol{r}\times\boldsymbol{p}$) is the angular momentum and $\boldsymbol{p}$ is the linear momentum.



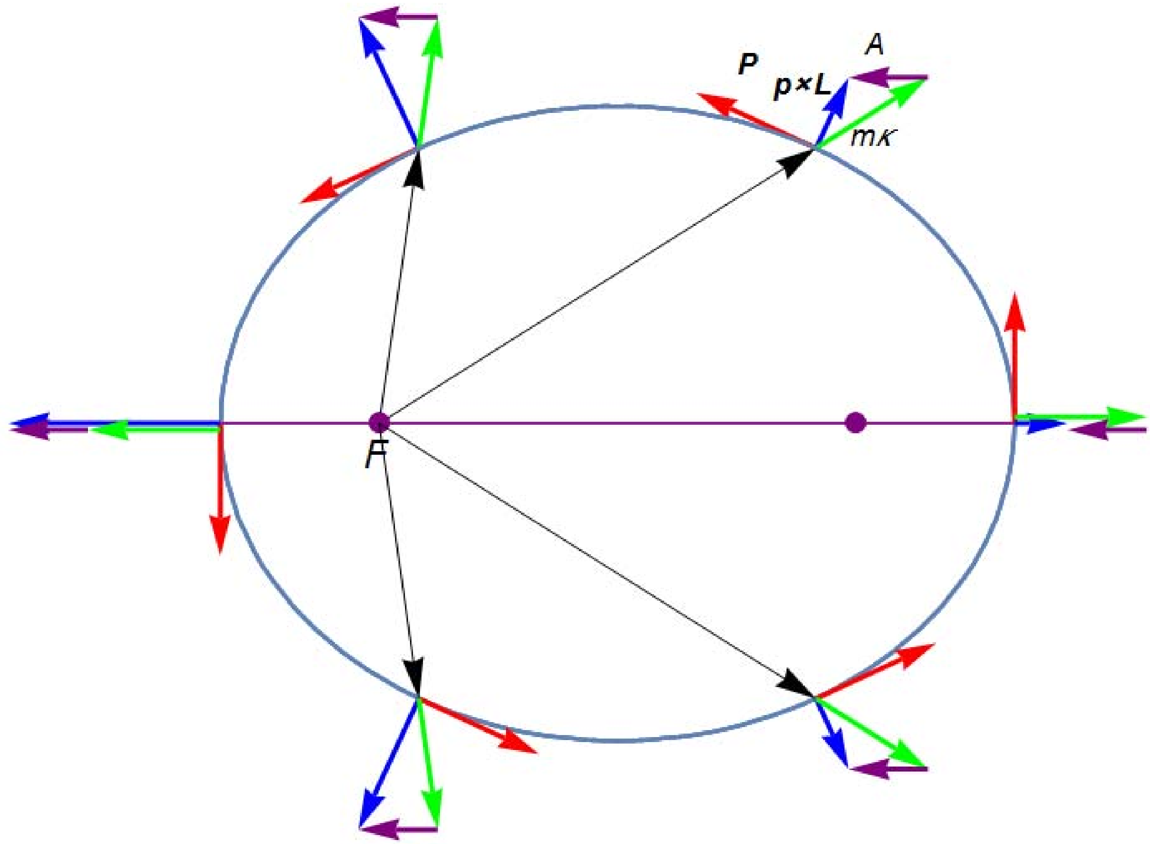


Fig. ***A*** *(=mM)* (denoted by the arrows with purple) on the ellipse orbits. The vector ***A*** points in the direction of the perihelion. The magnitude is constant. The angular momentum ***L*** is always perpendicular to the orbit. The perihelion, point of the orbit the nearest to the focal point F). The aphelion, the point of orbit from the focal point.

It is obvious from the definition that

$$\boldsymbol{L}\cdot\boldsymbol{M}=0, \qquad (\boldsymbol{M}\text{ lies in the plane of motion}).$$

$$\boldsymbol{p}\cdot\boldsymbol{M}=-\frac{\kappa}{r}\boldsymbol{p}\cdot\boldsymbol{r},$$

and

$$\begin{aligned}\boldsymbol{r}\cdot\boldsymbol{M} &= \boldsymbol{r}\cdot\left(-\frac{\kappa}{r}\boldsymbol{r}+\frac{1}{m}\boldsymbol{p}\times\boldsymbol{L}\right)\\ &= -\kappa r+\frac{1}{m}\boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L})\\ &= -\kappa r+\frac{1}{m}\boldsymbol{L}^2\\ &= -\kappa r+\frac{1}{m}l^2\end{aligned}.$$

or

$$\boldsymbol{r}\cdot\boldsymbol{A}=\boldsymbol{r}\cdot m\boldsymbol{M}=-m\kappa r+l^2,$$

since

$$\boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L})=\boldsymbol{L}\cdot(\boldsymbol{r}\times\boldsymbol{p})=\boldsymbol{L}^2,\qquad \boldsymbol{A}=m\boldsymbol{M}.$$

Since the angular momentum (along the *z* axis) is conserved, we can calculate

$$L=l=r_1p_1,$$

where p_1 is the linear momentum at the perihelion. $\boldsymbol{M}$ is a conserved quantity since

$$\begin{aligned}\frac{d}{dt}\boldsymbol{M} &= -\kappa\frac{d}{dt}\frac{1}{r}\boldsymbol{r}+\frac{1}{m}\frac{d}{dt}(\boldsymbol{p}\times\boldsymbol{L})\\ &= -\frac{\kappa}{m}\left[\frac{\boldsymbol{p}}{r}-\frac{\boldsymbol{r}(\boldsymbol{e}_r\cdot\boldsymbol{p})}{r^2}\right]+\frac{1}{m}[\boldsymbol{F}\times\boldsymbol{L}+\boldsymbol{p}\times(\boldsymbol{r}\times\boldsymbol{F})]\\ &= -\frac{\kappa}{m}\left[\frac{\boldsymbol{p}}{r}-\frac{\boldsymbol{r}(\boldsymbol{e}_r\cdot\boldsymbol{p})}{r^2}\right]-\frac{\kappa}{mr^2}[\boldsymbol{e}_r\times(\boldsymbol{r}\times\boldsymbol{p})+\boldsymbol{p}\times(\boldsymbol{r}\times\boldsymbol{e}_r)]\\ &= -\frac{\kappa}{m}\left[\frac{\boldsymbol{p}}{r}-\frac{\boldsymbol{r}(\boldsymbol{e}_r\cdot\boldsymbol{p})}{r^2}\right]-\frac{\kappa}{mr^2}[(\boldsymbol{e}_r\cdot\boldsymbol{p})\boldsymbol{r}-r\boldsymbol{p}+(\boldsymbol{p}\cdot\boldsymbol{e}_r)\boldsymbol{r}-(\boldsymbol{p}\cdot\boldsymbol{r})\boldsymbol{e}_r]\\ &= -\frac{\kappa}{m}\left[\frac{\boldsymbol{p}}{r}-\frac{\boldsymbol{r}(\boldsymbol{e}_r\cdot\boldsymbol{p})}{r^2}\right]-\frac{\kappa}{m}\left[-\frac{\boldsymbol{p}}{r}+\frac{(\boldsymbol{p}\cdot\boldsymbol{e}_r)\boldsymbol{r}}{r^2}\right]\\ &= 0\end{aligned}$$

where

$$\frac{d}{dt}\frac{1}{r}\boldsymbol{r}=\frac{1}{m}\left[\frac{\boldsymbol{p}}{r}-\frac{\boldsymbol{r}(\boldsymbol{e}_r\cdot\boldsymbol{p})}{r^2}\right],$$

$$\frac{d}{dt}\boldsymbol{p} = \boldsymbol{F} = -\frac{\kappa}{r^2}\boldsymbol{e}_r$$

and

$$\boldsymbol{\tau} = \frac{d}{dt}\boldsymbol{L} = r \times \boldsymbol{F} . \qquad \text{(torque).}$$

((**Mathematica**)) Proof of d$\boldsymbol{M}$/dt = 0.

```
Clear["Global`"]; r[t_] := {x[t], y[t], z[t]};
R[t_] := √(r[t].r[t]);

p[t_] := m D[r[t], t]; L[t_] := Cross[r[t], p[t]];
F[t_] := (-κ/R[t]^3) r[t];
eq1 =
  -κ D[r[t]/R[t], t] + 1/m (Cross[F[t], L[t]]) +
    1/m (Cross[p[t], Cross[r[t], F[t]]]) //
   FullSimplify
{0, 0, 0}
```

We note that

$$\boldsymbol{p} \times \boldsymbol{L} = \boldsymbol{p} \times (\boldsymbol{r} \times \boldsymbol{p}) = p^2\boldsymbol{r} - (\boldsymbol{p} \cdot \boldsymbol{r})\boldsymbol{p}$$

Then the vector $\boldsymbol{M}$ ($\boldsymbol{A} = m\boldsymbol{M}$) always points in the direction of the perihelion from the focal point. At the perihelion,

$$\boldsymbol{p} \cdot \boldsymbol{r} = 0$$

We have

$$
\begin{aligned}
\boldsymbol{A} &= m\boldsymbol{M} \\
&= -m\kappa \boldsymbol{e}_r + p^2 r_1 \boldsymbol{e}_r \\
&= (-m\kappa + \frac{l^2}{r_1})\boldsymbol{e}_r \\
&= (-m\kappa + \frac{l^2}{r_1})(-\boldsymbol{e}_x) \\
&= A_0(-\boldsymbol{e}_x)
\end{aligned}
$$

where $\boldsymbol{e}_r = -\boldsymbol{e}_x$ and

$$A_0 = -m\kappa + \frac{l^2}{r_1}.$$

In general case, we have the orbital equation as

$$\boldsymbol{r} \cdot \boldsymbol{A} = A_0 r \cos\chi = -m\kappa r + l^2,$$

where χ is the angle between $\boldsymbol{r}$ and the perihelion direction. From this equation we get

$$r(A_0 \cos\chi + m\kappa) = l^2,$$

or

$$r(\frac{A_0}{m\kappa}\cos\chi + 1) = \frac{l^2}{m\kappa}$$

$$r = \frac{\frac{l^2}{m\kappa}}{1 + \frac{A_0}{m\kappa}\cos\chi} = \frac{p_0}{1 + e\cos\chi},$$

Then we have p_0 is given by

$$p_0 = \frac{l^2}{m\kappa}. \qquad \text{(semi latus rectum)}$$

and

$$A = A_0 = m\kappa e.$$

Since $A_0 = -m\kappa + \frac{l^2}{r_1}$, we have

$$\frac{l^2}{r_1} = m\kappa(1+e)$$

3. Derivation of the Runge-Lentz vector

The equation of motion of a particle of mass m in the attractive potential is

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{F} = -\frac{\kappa}{r^2}\boldsymbol{e}_r .$$

We take the cross product of both sides with the angular momentum *L*.

$$\boldsymbol{L} \times \frac{d\boldsymbol{p}}{dt} = \boldsymbol{F} = -\frac{\kappa}{r^3}\boldsymbol{L} \times \boldsymbol{r} .$$

Since *L* is constant in time, the left-hand side can be written as

$$\boldsymbol{L} \times \frac{d\boldsymbol{p}}{dt} = \frac{d}{dt}(\boldsymbol{L} \times \boldsymbol{p}) .$$

From the explicit form

$$L = \boldsymbol{r} \times \boldsymbol{p} = m\boldsymbol{r} \times \frac{d\boldsymbol{r}}{dt},$$

we get

$$\begin{aligned} -\frac{\kappa}{r^3}\boldsymbol{L} \times \boldsymbol{r} &= \frac{\kappa}{r^3}\boldsymbol{r} \times \boldsymbol{L} = \frac{m\kappa}{r^3}\boldsymbol{r} \times (\boldsymbol{r} \times \frac{d\boldsymbol{r}}{dt}) \\ &= \frac{m\kappa}{r^3}[(\boldsymbol{r} \cdot \frac{d\boldsymbol{r}}{dt})\boldsymbol{r} - \boldsymbol{r}^2 \frac{d\boldsymbol{r}}{dt}] \\ &= -m\kappa \frac{d}{dt}\left(\frac{\boldsymbol{r}}{r}\right) \end{aligned}$$

Then we have

$$\frac{d}{dt}(\boldsymbol{L}\times\boldsymbol{p})+m\kappa\frac{d}{dt}\left(\frac{\boldsymbol{r}}{r}\right)=0,$$

or

$$\frac{d}{dt}(-\boldsymbol{L}\times\boldsymbol{p}-m\kappa\frac{\boldsymbol{r}}{r})=0.$$

The Runge-Lentz vector is obtained as

$$\boldsymbol{A}=m\boldsymbol{M}=-m\kappa\boldsymbol{e}_r-\boldsymbol{L}\times\boldsymbol{p}=-m\kappa\boldsymbol{e}_r+\boldsymbol{p}\times\boldsymbol{L}.$$

which is a constant of motion.

4. Energy of the system

We note that

$$\boldsymbol{M}^2=\frac{2H}{m}\boldsymbol{L}^2+\kappa^2.$$

The proof is given by using the Mathematica.

((**Mathematica**))

```
Clear["Global`"]; r = {x, y, z}; p = {px, py, pz};
L = Cross[r, p]; R = √(r.r);
M1 = (-κ/R) r + (1/m) Cross[p, L];

H1 = (1/(2 m)) p.p - κ/R;

eq1 = M1.M1 - (2/m) H1 (L.L) // FullSimplify
```

κ^2

The energy can be derived as follows.

$$\boldsymbol{A}^2 = m^2\boldsymbol{M}^2 = 2Hml^2 + m^2\kappa^2 = m^2\kappa^2 e^2,$$

or

$$H = E = -\frac{m\kappa^2}{2l^2}(1-e^2) = -\frac{\kappa}{2a} \qquad (<0),$$

with $A = m\kappa e$, $\boldsymbol{L}^2 = l^2$, and $H = E$.

4. Construction of the diagram by Mathematica

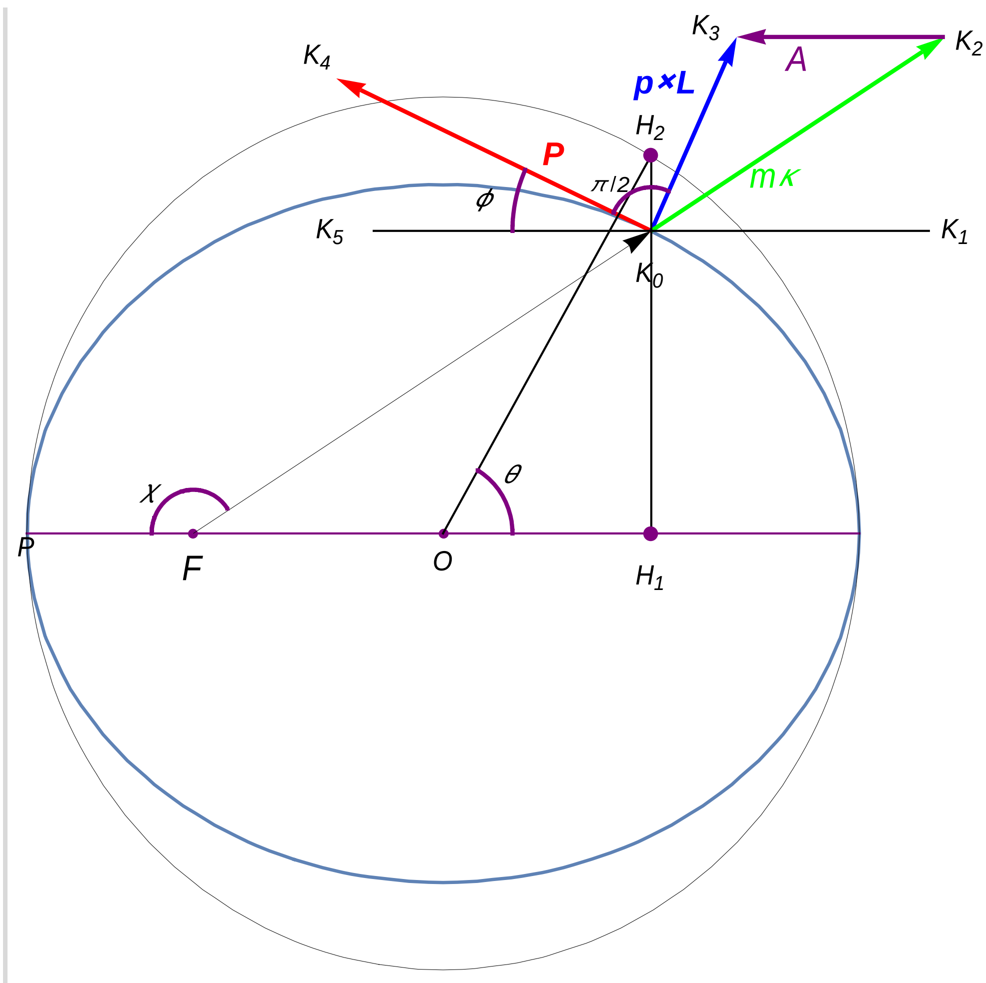


Fig. Simplified version of the diagram. χ is the angle between $\boldsymbol{A}$ and $\boldsymbol{r}$. The direction of A is from the focal point to the perihelion (P).

We consider a point (K_0) of the orbit of the ellipsoid which is expressed by

$$\frac{x^2}{a^2}+\frac{x^2}{b^2}=1,$$

where the essentricity ε is given by

$$e=\sqrt{1-\frac{b^2}{a^2}}.$$

where $a>b$. The co-ordinate of the focal point F is $(-ae,0)$. We also consider a point (H_2) on the circle which is expressed by

$$x^2+y^2=a^2.$$

We assume that the angle $\angle H_2OH_1$ is θ. The co-ordinates of the points K_0 and H_2

$$\overrightarrow{OH_2}=(a\cos\theta, a\sin\theta), \qquad \overrightarrow{OK_0}=(a\cos\theta, b\sin\theta).$$

The slope of the tangential line (K_0K_4) at the point K_0 on the ellipsoid is given by

$$\text{slope}=\frac{\frac{dy}{d\theta}}{\frac{dx}{d\theta}}=-\frac{b\cos\theta}{a\sin\theta}=-\frac{b}{a}\cot\theta=-\tan\phi,$$

where the angle $\angle K_4K_0K_1\phi$ is ϕ;

$$\phi=\arctan(\frac{b}{a}\cot\theta).$$

The unit vector along the vector $\overrightarrow{K_0K_2}$,

$$\boldsymbol{u}_2=\frac{\overrightarrow{K_0K_2}}{\left|\overrightarrow{K_0K_2}\right|}=\frac{(a\cos\theta+ae, b\sin\theta)}{\sqrt{(a\cos\theta+ae)^2+(b\sin\theta)^2}},$$

The unit vector along the vector $\overrightarrow{K_0K_2}$,

$$\boldsymbol{u}_3 = \frac{\overrightarrow{K_0 K_3}}{\left|\overrightarrow{K_0 K_3}\right|} = (\sin\phi, \cos\phi) .$$

We note that

$$\overrightarrow{K_0 K_3} = \boldsymbol{p} \times \boldsymbol{L} = s_3 \boldsymbol{u}_3 = \overrightarrow{K_0 K_2} + \overrightarrow{K_2 K_3} = m\kappa \boldsymbol{u}_2 - A\boldsymbol{e}_x ,$$

where

$$A = em\kappa , \qquad \boldsymbol{e}_x = (1,0).$$

Then we have

$$s_3 = m\kappa(\boldsymbol{u}_2 \cdot \boldsymbol{u}_3 - \boldsymbol{e}_x \cdot \boldsymbol{u}_3) .$$

The co-ordinate of the point is given by

$$\overrightarrow{OK_3} = \overrightarrow{OK_0} + \overrightarrow{K_0 K_3} = (a\cos\theta, b\sin\theta) + s_3 \boldsymbol{u}_3$$

((**Mathematica**))

```
Clear["Global`*"]; a = 3; b = 2.4; f1 = x^2/a^2 + y^2/b^2 == 1;
f2 = x^2 + y^2 == a^2; O1 = {0, 0}; e1 = Sqrt[1 - (b/a)^2]; s1 = 2.5;
s3 = 2.5; Q1 = {-a e1, 0}; Q2 = {a e1, 0}; A0 = e1 s3;
g1 = ContourPlot[Evaluate[f1], {x, -5, 5}, {y, -5, 5},
   Frame → None];
g2 = Graphics[{Purple, PointSize[0.01],
    Point[{Q1, O1}], Line[{{-a, 0}, {a, 0}}]}];
g3 = ContourPlot[Evaluate[f2], {x, -5, 5}, {y, -5, 5},
   ContourStyle → {Black, Thin}];
H1[θ1_] :=
 Module[{θ, ϕ1, A1, B1, C1, D1, G1, u1, u2, u3,
    ex, s2}, θ = θ1; ϕ1 = ArcTan[b/a Cot[θ]];
   ex = {1, 0};
   u1 = {- Cos[ϕ1] , Sin[ϕ1] };
   u2 = {Sin[ϕ1] , Cos[ϕ1] };
   u3 = {(a Cos[θ] + a e1)/Sqrt[(a Cos[θ] + a e1)^2 + (b Sin[θ])^2] ,
      b Sin[θ]/Sqrt[(a Cos[θ] + a e1)^2 + (b Sin[θ])^2]};
   C1 = {a Cos[θ], b Sin[θ]};
   s2 = -A0 (u2.ex) + s3 (u2.u3);
   A1 = s1 u1 + C1;
   B1 = s2 u2 + C1;
   D1 = s3 u3 + C1;
```

```
  Graphics[{Black, Thin, Arrowheads[0.030],
    Arrow[{Q1, C1}], Red, Thick, Arrow[{C1, A1}],
    Blue, Arrow[{C1, B1}], Green, Arrow[{C1, D1}],
    Purple, Arrow[{D1, B1}]}]]; θ2 = 60 °;
h1 = Show[g1, g2, g3, H1[θ2]];
h2 =
 Graphics[
  {Text[Style["P", Italic, 15, Red, Bold],
    {0.8, 2.6}],
   Text[Style["p×L", Italic, Blue, 15, Bold],
    {1.6, 3.1}], Text[Style["mκ", Italic, Green, 15],
    {2.4, 2.45}], Text[Style["A", Italic, Purple, 15],
    {2.55, 3.25}], Text[Style["F", Italic, 15],
    {-a e1, -0.25}],
   Text[Style["θ", Italic, 12], {0.5, 0.4}],
   Text[Style["ϕ", Italic, 12], {0.3, 2.3}],
   Text[Style["π/2", Italic, 10], {1.2, 2.4}],
   Text[Style["O", Italic, 12], {0, -0.2}],
   Text[Style["H1", Italic, 12], {a Cos[θ2], -0.3}],
   Text[Style["H2", Italic, 12],
    {a Cos[θ2], a Sin[θ2] + 0.2}],
   Text[Style["K0", Italic, 12],
    {a Cos[θ2], b Sin[θ2] - 0.3}],
   Text[Style["K1", Italic, 12],
    {a Cos[θ2] + 2.2, b Sin[θ2]}],
   Text[Style["K2", Italic, 12],
    {a Cos[θ2] + 2.3, b Sin[θ2] + 1.3}],
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    Text[Style["K₃", Italic, 12],
     {a Cos[θ2] + 0.4, b Sin[θ2] + 1.4}],
    Text[Style["K₄", Italic, 12],
     {a Cos[θ2] - 2.4, b Sin[θ2] + 1.2}],
    Text[Style["K₅", Italic, 12],
     {a Cos[θ2] - 2.3, b Sin[θ2] + 0}]}];
h3 =
 Graphics[
  {Line[{{a Cos[θ2], 0}, {a Cos[θ2], a Sin[θ2]}}],
   Line[{O1, {a Cos[θ2], a Sin[θ2]}}],
   Line[{{a Cos[θ2], b Sin[θ2]} + {-2, 0},
     {a Cos[θ2], b Sin[θ2]} + {2, 0}}]}]; r2 = 1;
r3 = 0.3; ϕ2 = ArcTan[b/a Cot[θ2]];
h4 = ParametricPlot[
  {r2 Cos[θ] + a Cos[θ2], r2 Sin[θ] + b Sin[θ2]},
  {θ, π - ϕ2, π}, PlotStyle → {Purple, Thick}];
h5 = ParametricPlot[{0.5 Cos[θ] , 0.5 Sin[θ]},
  {θ, 0, θ2}, PlotStyle → {Purple, Thick}];
h6 = ParametricPlot[
  {r3 Cos[θ] + a Cos[θ2], r3 Sin[θ] + b Sin[θ2]},
  {θ, π / 2 - ϕ2, π - ϕ2}, PlotStyle → {Purple, Thick}];
H1 = {a Cos[θ2], 0}; H2 = {a Cos[θ2], a Sin[θ2]};
h7 = Graphics[{Purple, PointSize[0.015],
   Point[{H1, H2}]}];
Show[h1, h2, h3, h4, h5, h6, h7, PlotRange → All]
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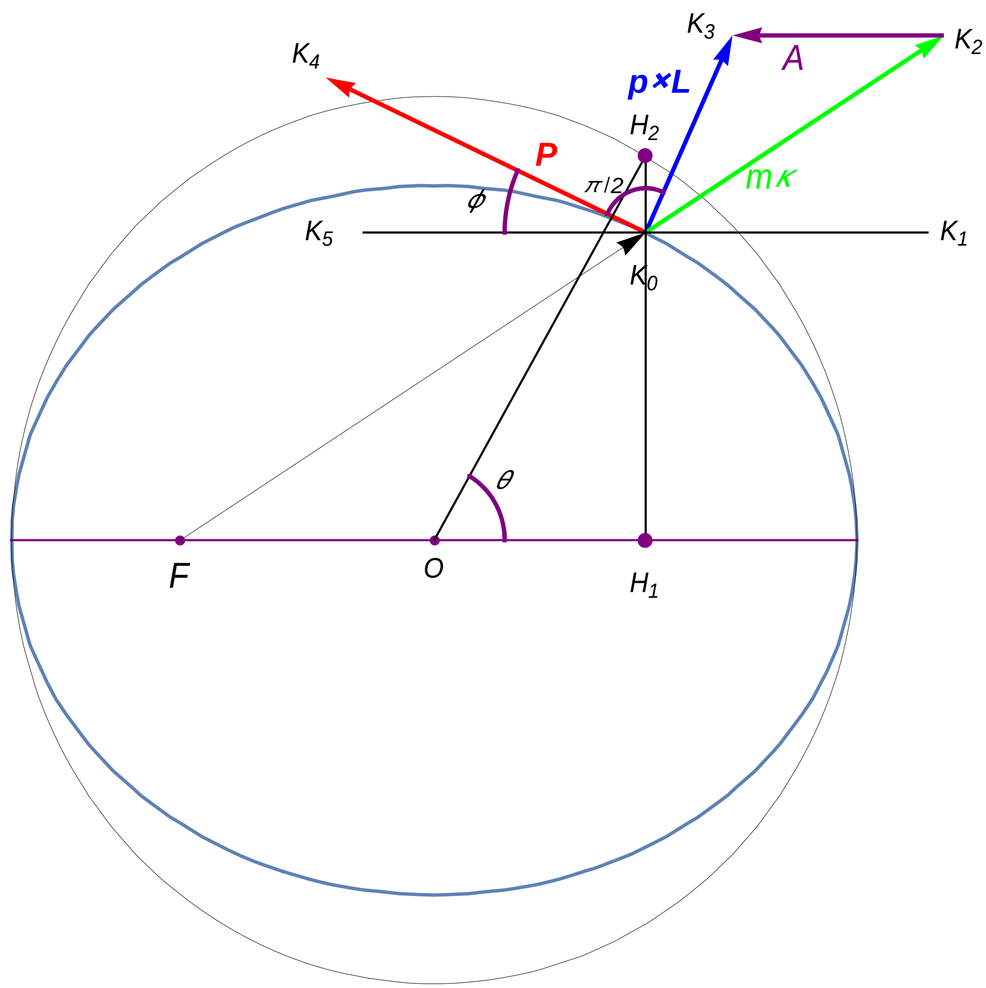

5 Invariance of H under the rotation

Suppose that the Hamiltonian (with the spherical symmetry) is given by

$$\hat{H} = \frac{1}{2m}\hat{\boldsymbol{p}}^2 - \frac{Ze^2}{|\hat{\boldsymbol{r}}|}$$

in our system, we consider the infinitesimal rotation

$$|\psi'\rangle = \hat{R}(\varepsilon)|\psi\rangle .$$

If $\hat{H}$ is invariant under the rotation,

$$\langle\psi'|\hat{H}|\psi'\rangle = \langle\psi|\hat{H}|\psi\rangle ,$$

or

$$\langle\psi|\hat{R}^{+}(\varepsilon)\hat{H}\hat{R}(\varepsilon)|\psi\rangle = \langle\psi|\hat{H}|\psi\rangle,$$

or

$$\hat{R}^{+}(\varepsilon)\hat{H}\hat{R}(\varepsilon) = \hat{H},$$

or

$$\hat{H}\hat{R}(\varepsilon) = \hat{R}(\varepsilon)\hat{H},$$

or

$$[\hat{R}(\varepsilon), \hat{H}] = 0.$$

Since $\hat{R}(\varepsilon) = 1 - \frac{i}{\hbar}(\hat{\boldsymbol{L}}.\boldsymbol{n})\varepsilon$, we obtain the following commutation relations.

$$[\hat{H}, \hat{\boldsymbol{L}}.\boldsymbol{n}] = 0.$$

Since $\boldsymbol{n}$ is any unit vector ,

$$[\hat{H}, \hat{L}_x] = \hat{0}, \qquad [\hat{H}, \hat{L}_y] = \hat{0}, \qquad [\hat{H}, \hat{L}_z] = \hat{0}.$$

and

$$[\hat{H}, \hat{L}_x{}^2] = \hat{0}, \qquad [\hat{H}, \hat{L}_y{}^2] = \hat{0}, \qquad [\hat{H}, \hat{L}_z{}^2] = \hat{0}.$$

Hereafter, We use the notation such that

$$\langle\boldsymbol{r}|\hat{H}|\psi\rangle = H\psi(\boldsymbol{r}).$$

$$\langle\boldsymbol{r}|\hat{\boldsymbol{L}}|\psi\rangle = \boldsymbol{L}\psi(\boldsymbol{r})$$

where H and $\boldsymbol{L}$ are differential operators.

5. Runge-Lenz vector in quantum mechanics

Here we introduce a Runge-Lenz vector which in quantum mechanics is defined by

$$\boldsymbol{M} = -\frac{Ze^2}{r}\boldsymbol{r} + \frac{1}{2m}(\boldsymbol{p}\times\boldsymbol{L} - \boldsymbol{L}\times\boldsymbol{p}) .$$

This operator is Hermitian since $(\boldsymbol{p}\times\boldsymbol{L})^{+} = -(\boldsymbol{L}\times\boldsymbol{p})$ Note that $\boldsymbol{r}$ [=(x, y, z)] is the position vector, $\boldsymbol{L}$ is the orbital angular momentum,

$$\boldsymbol{L} = \boldsymbol{r}\times\boldsymbol{p} .$$

$\boldsymbol{M}$ commutes with the Hamiltonian H (the proof is given using Mathematica)

$$[H, M_i] = 0 ,$$

where H is the Coulomb Hamiltonian

$$H = \frac{1}{2m}\boldsymbol{p}^2 - \frac{Ze^2}{r} .$$

We also have

$$[H, M_i^{\,2}] = [H, M_i]M_i + M_i[H, M_i] = 0$$

The commutation relations between the angular momentum $\boldsymbol{L}$ and linear momentum $\boldsymbol{p}$ are given by

$$[L_i, p_j] = i\hbar\varepsilon_{ijk}p_k ,$$

which leads to the expression

$$\boldsymbol{L}\times\boldsymbol{p} + \boldsymbol{p}\times\boldsymbol{L} = 2i\hbar\boldsymbol{p} .$$

Then we have

$$\boldsymbol{M} = -\frac{Ze^2}{r}\boldsymbol{r} + \frac{1}{m}(\boldsymbol{p}\times\boldsymbol{L}) - \frac{i\hbar}{m}\boldsymbol{p} .$$

We note that

$$\boldsymbol{L}\cdot\boldsymbol{M}=\boldsymbol{M}\cdot\boldsymbol{L}=0.$$

(the proof is given using the Matheamtica). We also note that

$$\boldsymbol{r}\cdot(\boldsymbol{p}\times\boldsymbol{L})=\boldsymbol{L}^2, \qquad (\boldsymbol{p}\times\boldsymbol{L})\cdot\boldsymbol{r}=\boldsymbol{L}^2+2i\hbar\boldsymbol{p}\cdot\boldsymbol{r},$$

$$(\boldsymbol{p}\times\boldsymbol{L})^2=\boldsymbol{p}^2\boldsymbol{L}^2.$$

We find that

$$\boldsymbol{M}^2=Z^2e^4+\frac{2}{m}H(\boldsymbol{L}^2+\hbar^2).$$

The $\hbar^2$ term arises from the non-commutativity of quantum operators. These equations can be easily proved using the Mathematica (see below in detail).

We know that the angular momentum operators satisfy the commutation relations,

$$[L_i,L_j]=i\hbar\varepsilon_{ijk}L_k.$$

We also get

$$[M_i,L_j]=i\hbar\varepsilon_{ijk}M_k,$$

and

$$[M_i,M_j]=-\frac{2i\hbar}{m}\varepsilon_{ijk}HL_k.$$

The L_i's generate rotations and define a closed algebra. But L_i.s and M_i's do not form a closed algebra since the last relation involves the Hamiltonian. However, we consider the case of specific bound states. In this case, the vector space is truncated only those that are eigenstates of *H*, with eigenvalue *E*<0. In this case we replace *H* with –*E*, and the algebra is closed.

We define a new vector ***N*** such that

$$\boldsymbol{N}=(-\frac{m}{2E})^{1/2}\boldsymbol{M}.$$

where $H\rightarrow -E$ with $E<0$. In this case we have the closed algebra,

$$[L_i, L_j] = i\hbar\varepsilon_{ijk} L_k \,,$$

$$[N_i, L_j] = i\hbar\varepsilon_{ijk} N_k \,, \quad \text{or} \quad [L_i, N_j] = i\hbar\varepsilon_{ijk} N_k$$

and

$$[N_i, N_j] = i\hbar\varepsilon_{ijk} L_k \,,$$

$$[M_i, \boldsymbol{L}^2] \neq 0 \,.$$

In the present notation, we have

$$[L_i, H] = 0 \,, \quad [L_i{}^2, H] = L_i[L_i, H] + [L_i, H]L_i = 0$$

and

$$[N_i, H] = 0 \,, \quad [N_i{}^2, H] = N_i[N_i, H] + [N_i, H]N_i = 0$$

8. Dynamic Symmetry operation

We consider the symmetry operation generated by the operators ***L*** and ***N***, which corresponds to the rotation in four spatial dimensions. We introduce (x_1, x_2, x_3, x_4) and (p_1, p_2, p_3, p_4). Note that x_4 and p_4 are fictitious and cannot be identified with dynamical variables.

$$L_1 = L_x = L_{23} = x_2 p_3 - x_3 p_2 \,,$$

$$L_2 = L_y = L_{31} = x_3 p_1 - x_1 p_3 \,,$$

$$L_3 = L_z = L_{12} = x_1 p_2 - x_2 p_1 \,,$$

$$N_1 = L_{14} = x_1 p_4 - x_4 p_1 \,,$$

$$N_2 = L_{24} = x_2 p_4 - x_4 p_2 \,,$$

$$N_3 = L_{34} = x_3 p_4 - x_4 p_3 \,.$$

This algebra is isomorphic (equivalent) to that of rotations in four dimensions [or the SO(4) group].

9. New operators I_i and K_i

We define two sets of new generators as

$$I_i = \frac{1}{2}(L_i + N_i), \qquad K_i = \frac{1}{2}(L_i - N_i).$$

and

$$L_i = I_i + K_i .$$

Then we get

$$[I_i, I_j] = i\hbar\varepsilon_{ijk} I_k , \qquad \boldsymbol{I}\times\boldsymbol{I} = i\hbar\boldsymbol{I}$$

$$[K_i, K_j] = i\hbar\varepsilon_{ijk} K_k , \qquad \boldsymbol{K}\times\boldsymbol{K} = i\hbar\boldsymbol{K}$$

$$[I_i, K_j] = 0 .$$

since

$$\begin{aligned}
[I_1, I_2] &= \frac{1}{4}[L_1 + N_1, L_2 + N_2] \\
&= \frac{1}{4}\{[L_1, L_2] + [L_1, N_2] + [N_1, L_2] + [N_{1,} N_2]\} \\
&= \frac{1}{4}(i\hbar L_3 + i\hbar N_3 + i\hbar N_3 + i\hbar L_3) \\
&= i\hbar\frac{1}{2}(L_3 + N_3) \\
&= i\hbar I_3
\end{aligned}$$

$$
\begin{aligned}
[K_1, K_2] &= \frac{1}{4}[L_1 - N_1, L_2 - N_2] \\
&= \frac{1}{4}\{[L_1, L_2] - [L_1, N_2] - [N_1, L_2] + [N_1, N_2]\} \\
&= \frac{1}{4}(i\hbar L_3 - i\hbar N_3 - i\hbar N_3 + i\hbar L_3) \\
&= i\hbar \frac{1}{2}(L_3 - N_3) \\
&= i\hbar K_3
\end{aligned}
$$

$$
\begin{aligned}
[I_1, K_2] &= \frac{1}{4}[L_1 + N_1, L_2 - N_2] \\
&= \frac{1}{4}\{[L_1, L_2] - [L_1, N_2] + [N_1, L_2] - [N_1, N_2]\} \\
&= \frac{1}{4}(i\hbar L_3 - i\hbar N_3 + i\hbar N_3 - i\hbar L_3) \\
&= 0
\end{aligned}
$$

We have two Casimir operators $\boldsymbol{I}^2$ and $\boldsymbol{K}^2$ or any combination of them; for example

$$
\boldsymbol{I}^2 = \boldsymbol{K}^2 = \frac{1}{4}(\boldsymbol{L}^2 + \boldsymbol{N}^2)
$$

since

$$
\boldsymbol{I}^2 = \frac{1}{4}(\boldsymbol{L}^2 + \boldsymbol{N}^2 + \boldsymbol{L}\cdot\boldsymbol{N} + \boldsymbol{N}\cdot\boldsymbol{L}) = \frac{1}{4}(\boldsymbol{L}^2 + \boldsymbol{N}^2)
$$

where

$$
\boldsymbol{L}\cdot\boldsymbol{N} = (-\frac{m}{2E})^{1/2}\boldsymbol{L}\cdot\boldsymbol{M} = 0, \qquad \boldsymbol{N}\cdot\boldsymbol{L} = (-\frac{m}{2E})^{1/2}\boldsymbol{M}\cdot\boldsymbol{L} = 0
$$

with

$$
\boldsymbol{N} = (-\frac{m}{2E})^{1/2}\boldsymbol{M}
$$

We also have the commutation relations

$$[\boldsymbol{I}^2, I_k] = 0, \qquad [\boldsymbol{K}^2, K_k] = 0$$

$$[\boldsymbol{K}^2, I_k] = 0, \qquad [\boldsymbol{I}^2, K_k] = 0$$

10. Eigenvalue of Hamiltonian

We also have the following commutation relations

$$[I_i, H] = [K_i, H] = 0 .$$

and

$$[I_i^2, H] = [K_i^2, H] = 0$$

since

$$[I_i, H] = \frac{1}{2}[L_i + N_i, H] = 0, \qquad [K_i, H] = \frac{1}{2}[L_i - N_i, H] = 0$$

So that these operators are also conserved. In this basis the algebra becomes equivalent to that of two decoupled algebras of angular momenta. The eigenvalues of the operators $\boldsymbol{I}^2$ and $\boldsymbol{K}^2$ will have the eigenvalues,

$$\boldsymbol{I}^2; \quad \hbar^2 i(i+1), \qquad \boldsymbol{K}^2; \quad \hbar^2 k(k+1) .$$

where *i* and *k* are either integer or half integers. We note that

$$C = \boldsymbol{I}^2 + \boldsymbol{K}^2 = \frac{1}{2}(\boldsymbol{L}^2 + \boldsymbol{N}^2),$$

$$C' = \boldsymbol{I}^2 - \boldsymbol{K}^2 = \boldsymbol{L}.\boldsymbol{N} = 0 .$$

The second relation implies that

$$i(i+1) = k(k+1),$$

or

$i = k$.

Correspondingly, the allowed values of C are

$$C: \qquad 2\hbar^2 k(k+1),$$

$$\boldsymbol{M}^2 = -\frac{2E}{m}\boldsymbol{N}^2 = Z^2e^4 - \frac{2}{m}E(\boldsymbol{L}^2 + \hbar^2),$$

or

$$\boldsymbol{N}^2 = -\frac{mZ^2e^4}{2E} - (\boldsymbol{L}^2 + \hbar^2),$$

or

$$\frac{1}{2}(\boldsymbol{L}^2 + \boldsymbol{N}^2) = -\frac{mZ^2e^4}{4E} - \frac{\hbar^2}{2} = 2\hbar^2 k(k+1),$$

or

$$-\frac{mZ^2e^4}{4E} = \frac{\hbar^2}{2}[4k(k+1)+1] = \frac{\hbar^2}{2}(2k+1)^2,$$

$$E = -\frac{mZ^2e^4}{2\hbar^2(2k+1)^2} = -\frac{mZ^2e^4}{2\hbar^2 n^2}$$. (energy level of hydrogen atom).

where

$$n = 2k+1.$$

Since $\boldsymbol{L} = \boldsymbol{I} + \boldsymbol{K}$ with $i = k$,

$l = i + k, i + k - 1, \ldots, |l - k|$,

or

$l = 2k, 2k - 1, \ldots, 0$.

or

$l = n - 1, n - 2, \ldots\ldots.., 0.$

---

8. Proof of formula by using Mathematica

(1)

$$\boldsymbol{M} \cdot \boldsymbol{L} = 0, \qquad \boldsymbol{L} \cdot \boldsymbol{M} = 0$$

(2)

$$[M_i, \boldsymbol{L}^2] \neq 0$$

(3)

$$\boldsymbol{r}.(\boldsymbol{p} \times \boldsymbol{L}) = \boldsymbol{L}^2, \qquad (\boldsymbol{p} \times \boldsymbol{L}) \cdot \boldsymbol{r} = \boldsymbol{L}^2 + 2i\hbar(\boldsymbol{p} \cdot \boldsymbol{r})$$

(4)

$$\boldsymbol{p}.(\boldsymbol{p} \times \boldsymbol{L}) = 0$$

(5)

$$(\boldsymbol{p} \times \boldsymbol{L}) \cdot \boldsymbol{p} = 2i\hbar \boldsymbol{p}^2$$

(6)

$$[H, M_i] = 0$$

(7)

$$\boldsymbol{M}^2 - Z^2 e^4 = \frac{2}{m} H(\boldsymbol{L}^2 + \hbar^2)$$

(8)

$$[L_x, L_y] = i\hbar L_z, \qquad [M_x, L_y] = i\hbar M_z, \qquad [M_y, L_z] = i\hbar M_x$$

(9)

$$[M_x, M_y] = -i\frac{2\hbar}{m}HL_z$$

$$[M_y, M_z] = -i\frac{2\hbar}{m}HL_x$$

((**Mathematica**))

```
Clear["Global`"];

ux = {1, 0, 0}; uy = {0, 1, 0}; uz = {0, 0, 1}; r = {x, y, z};
R = Sqrt[x^2 + y^2 + z^2];

L := -ⅈ ℏ Cross[r, Grad[#, {x, y, z}]] & // Simplify;
P := -ⅈ ℏ Grad[#, {x, y, z}] &; Lx := ux.L[#] &; Ly := uy.L[#] &;
Lz := uz.L[#] &; Px := ux.P[#] &; Py := uy.P[#] &;
Pz := uz.P[#] &; PSQ := (Px[Px[#]] + Py[Py[#]] + Pz[Pz[#]]) &;
LSQ := (Lx[Lx[#]] + Ly[Ly[#]] + Lz[Lz[#]]) &;
```

$$Mx := \left(\frac{1}{m}\,(Py[Lz[\#]] - Pz[Ly[\#]]) - \frac{i\hbar}{m}\,Px[\#] - \frac{Z1\, e1^2}{R}\, x\, \#\right) \&;$$

$$My := \left(\frac{1}{m}\,(Pz[Lx[\#]] - Px[Lz[\#]]) - \frac{i\hbar}{m}\,Py[\#] - \frac{Z1\, e1^2}{R}\, y\, \#\right) \&;$$

$$Mz := \left(\frac{1}{m}\,(Px[Ly[\#]] - Py[Lx[\#]]) - \frac{i\hbar}{m}\,Pz[\#] - \frac{Z1\, e1^2}{R}\, z\, \#\right) \&;$$

```
M1 = (ux Mx[#] + uy My[#] + uz Mz[#]) &;
```

Proof

Mx Lx + My Ly + Mz Lz = 0

```
Mx[Lx[ψ[x, y, z]]] + My[Ly[ψ[x, y, z]]] + Mz[Lz[ψ[x, y, z]]] //
  FullSimplify

0
```

Proof

Lx Mx + Ly My + Lz Mz = 0

```
Lx[Mx[ψ[x, y, z]]] + Ly[My[ψ[x, y, z]]] + Lz[Mz[ψ[x, y, z]]] //
  FullSimplify

0
```

Proof

$[M_i, L^2] \neq 0$

Mx[LSQ[ψ[x, y, z]]] - LSQ[Mx[ψ[x, y, z]]] // Simplify

$$-\frac{1}{m} 2 \hbar^2 \left(-\frac{e1^2 \, m \, x \, Z1 \, \psi[x, y, z]}{\sqrt{x^2 + y^2 + z^2}} - \frac{e1^2 \, m \, x \, z \, Z1 \, \psi^{(0,0,1)}[x, y, z]}{\sqrt{x^2 + y^2 + z^2}} + x \hbar^2 \psi^{(0,0,2)}[x, y, z] - \frac{e1^2 \, m \, x \, y \, Z1 \, \psi^{(0,1,0)}[x, y, z]}{\sqrt{x^2 + y^2 + z^2}} + x \hbar^2 \psi^{(0,2,0)}[x, y, z] + \frac{e1^2 \, m \, y^2 \, Z1 \, \psi^{(1,0,0)}[x, y, z]}{\sqrt{x^2 + y^2 + z^2}} + \frac{e1^2 \, m \, z^2 \, Z1 \, \psi^{(1,0,0)}[x, y, z]}{\sqrt{x^2 + y^2 + z^2}} - \hbar^2 \psi^{(1,0,0)}[x, y, z] - 3 z \hbar^2 \psi^{(1,0,1)}[x, y, z] + x^2 \hbar^2 \psi^{(1,0,2)}[x, y, z] + y^2 \hbar^2 \psi^{(1,0,2)}[x, y, z] - 3 y \hbar^2 \psi^{(1,1,0)}[x, y, z] - 2 y z \hbar^2 \psi^{(1,1,1)}[x, y, z] + x^2 \hbar^2 \psi^{(1,2,0)}[x, y, z] + z^2 \hbar^2 \psi^{(1,2,0)}[x, y, z] - 2 x \hbar^2 \psi^{(2,0,0)}[x, y, z] - 2 x z \hbar^2 \psi^{(2,0,1)}[x, y, z] - 2 x y \hbar^2 \psi^{(2,1,0)}[x, y, z] + y^2 \hbar^2 \psi^{(3,0,0)}[x, y, z] + z^2 \hbar^2 \psi^{(3,0,0)}[x, y, z] \right)$$

Proof

$x \, (P \times L)_x + y \, (P \times L)_y + z \, (P \times L)_z = L^2$

```
x (Py[Lz[ψ[x, y, z]]] - Pz[Ly[ψ[x, y, z]]]) +
  y (Pz[Lx[ψ[x, y, z]]] - Px[Lz[ψ[x, y, z]]]) +
  z (Px[Ly[ψ[x, y, z]]] - Py[Lx[ψ[x, y, z]]]) -
  Lx[Lx[ψ[x, y, z]]] - Ly[Ly[ψ[x, y, z]]] -
  Lz[Lz[ψ[x, y, z]]] // FullSimplify

0
```

Proof

$(P \times L)_x\, x + (P \times L)_y\, y + (P \times L)_z\, z = L^2 + 2\, i\, \hbar\, (Px\, x + Py\, y + Pz\, z)$

```
(Py[Lz[x ψ[x, y, z]]] - Pz[Ly[x ψ[x, y, z]]]) +
  (Pz[Lx[y ψ[x, y, z]]] - Px[Lz[y ψ[x, y, z]]]) +
  (Px[Ly[z ψ[x, y, z]]] - Py[Lx[z ψ[x, y, z]]]) -
  Lx[Lx[ψ[x, y, z]]] - Ly[Ly[ψ[x, y, z]]] - Lz[Lz[ψ[x, y, z]]] -
  2 ⅈ ℏ Px[x ψ[x, y, z]] - 2 ⅈ ℏ Py[y ψ[x, y, z]] -
  2 ⅈ ℏ Pz[z ψ[x, y, z]] // FullSimplify

0
```

Proof

$Px\,(P \times L)_x + Py\,(P \times L)_y + Pz\,(P \times L)_z = 0$

P. (**P** x **L**)=0

```
Px[Py[Lz[ψ[x, y, z]]]] - Px[Pz[Ly[ψ[x, y, z]]]] +
  Py[Pz[Lx[ψ[x, y, z]]]] - Py[Px[Lz[ψ[x, y, z]]]] +
  Pz[Px[Ly[ψ[x, y, z]]]] - Pz[Py[Lx[ψ[x, y, z]]]] //
 FullSimplify
```

```
0
```

Proof

$(P \times L)_x$ Px + $(P \times L)_y$ Py + $(P \times L)_z$ Pz = $2\,i\,\hbar\,(Px^2 + Py^2 + Pz^2)$

$(\mathbf{P} \times \mathbf{L}).\,\mathbf{P}. = 2\,i\,\hbar\,P^2$

```
Py[Lz[Px[ψ[x, y, z]]]] - Pz[Ly[Px[ψ[x, y, z]]]] +
  Pz[Lx[Py[ψ[x, y, z]]]] - Px[Lz[Py[ψ[x, y, z]]]] +
  Px[Ly[Pz[ψ[x, y, z]]]] - Py[Lx[Pz[ψ[x, y, z]]]] -
  2 i ℏ (Px[Px[ψ[x, y, z]]] + Py[Py[ψ[x, y, z]]] +
     Pz[Pz[ψ[x, y, z]]]) // FullSimplify
```

```
0
```

Proof

$(\boldsymbol{P} \times \boldsymbol{L})^2 = \mathbf{P}^2 \mathbf{L}^2$

```
K1 = Py[Lz[Py [Lz[ψ[x, y, z]]]]] - Py[Lz[Pz [Ly[ψ[x, y, z]]]]] -
     Pz[ Ly[Py[ Lz[ψ[x, y, z]]]]] + Pz[Ly[Pz[Ly[ψ[x, y, z]]]]] +
     Pz[Lx[Pz[Lx[ψ[x, y, z]]]]] - Pz[Lx[Px [Lz[ψ[x, y, z]]]]] -
     Px[ Lz[Pz[Lx[ψ[x, y, z]]]]] + Px[Lz[Px [Lz[ψ[x, y, z]]]]] +
     Px[Ly[Px[Ly[ψ[x, y, z]]]]] - Px[Ly[Py [Lx[ψ[x, y, z]]]]] -
     Py[ Lx[Px[Ly[ψ[x, y, z]]]]] + Py[Lx[Py [Lx[ψ[x, y, z]]]]] //
    FullSimplify;

K2 = PSQ[LSQ[ψ[x, y, z]]] // Simplify;

K1 - K2 // Simplify

0
```

Definition of Hamiltonian

$$H = \frac{1}{2m}(Px^2 + Py^2 + Pz^2) - \frac{Z^2 e^2}{r}$$

```
H1 := (1/(2 m) PSQ[#] - (Z1 e1^2)/R #) &;
```

Proof [H, Mx]=0, [H, My]=0, [H, My]=0,

```
H1[Mx[ψ[x, y, z]]] - Mx[H1[ψ[x, y, z]]] // FullSimplify
0
```

```
H1[My[ψ[x, y, z]]] - My[H1[ψ[x, y, z]]] // FullSimplify
0
```

Proof $Mx^2 + My^2 + Mz^2 - Z^2 e^4 = \frac{2}{m} H (L^2 + \hbar^2)$

```
MSQ1 = Mx[Mx[ψ[x, y, z]]] + My[My[ψ[x, y, z]]] +
    Mz[Mz[ψ[x, y, z]]] - Z1^2 e1^4 ψ[x, y, z] // Simplify;
```

```
eq1 = 2/m (H1[LSQ[ψ[x, y, z]]] + ħ^2 H1[ψ[x, y, z]]);
```

```
MSQ1 - eq1 // FullSimplify
0
```

Proof

[Lx, Ly] = i ℏ Lz,

[Mx, Ly] = i ℏ Mz,

[My, Lz] = i ℏ Mx,

```
Lx[Ly[ψ[x, y, z]]] - Ly[Lx[ψ[x, y, z]]] - ⅈ ℏ Lz[ψ[x, y, z]] //
 Simplify
```

0

```
Mx[Ly[ψ[x, y, z]]] - Ly[Mx[ψ[x, y, z]]] - ⅈ ℏ Mz[ψ[x, y, z]] //
 Simplify
```

0

```
My[Lz[ψ[x, y, z]]] - Lz[My[ψ[x, y, z]]] - ⅈ ℏ Mx[ψ[x, y, z]] //
 Simplify
```

0

Proof

[Mx, My] =- i $\frac{2\hbar}{m}$ H Lz,

[My, Mz] =- i $\frac{2\hbar}{m}$ H Lx,

```
Mx[My[ψ[x, y, z]]] - My[Mx[ψ[x, y, z]]] +
   ⅈ (2 ℏ)/m H1[Lz[ψ[x, y, z]]] // Simplify
```

0

```
My[Mz[ψ[x, y, z]]] - Mz[My[ψ[x, y, z]]] +
   ⅈ (2 ℏ)/m H1[Lx[ψ[x, y, z]]] // Simplify
```

0

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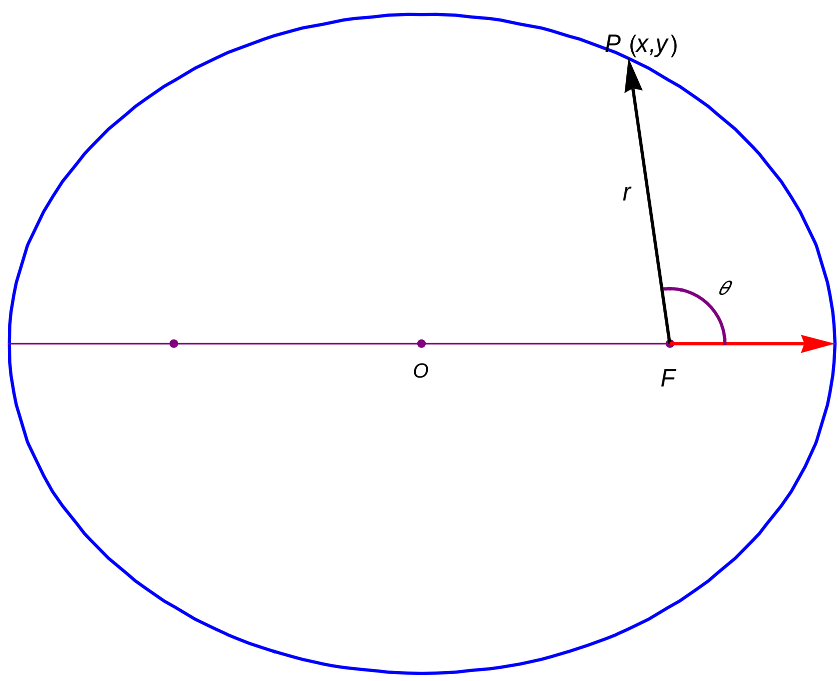
APPENDIX Kepler's law

For convenience, we use the following diagram for the ellipse orbit.



A.1 The angular momentum

In general case

$$a_r = \ddot{r} - r\dot{\theta}^2$$
$$a_\theta = r\ddot{\theta} + 2\dot{r}\dot{\theta} = \frac{1}{r}\frac{d}{dt}(r^2\dot{\theta})$$
$$v_r = \dot{r}$$
$$v_\theta = r\dot{\theta}$$

Since the gravitational force is directed toward the origin (so called central field),

$$ma_r = -G\frac{Mm}{r^2} = -\frac{\kappa}{r^2}$$
$$ma_\theta = 0$$

where

$$\kappa = mMG \, .$$

In other words,

$$a_\theta = r\ddot{\theta} + 2\dot{r}\dot{\theta} = \frac{1}{r}\frac{d}{dt}(r^2\dot{\theta}) = 0$$
$$v_\theta = r\dot{\theta}$$

or

$$l = mr^2\dot{\theta} = mr^2\frac{v_\theta}{r} = mrv_\theta = \text{constant}.$$

The angular momentum is defined as

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{r} \times (m\boldsymbol{v}) = m(r\boldsymbol{e}_r) \times (v_r\boldsymbol{e}_r + v_\theta\boldsymbol{e}_\theta) = mrv_\theta\boldsymbol{e}_z = L_z\boldsymbol{e}_z \, ,$$

or

$$L_z = mv_\theta r \, ,$$

$$\frac{d\boldsymbol{L}}{dt} = \frac{d}{dt}(\boldsymbol{r} \times \boldsymbol{p}) = \frac{d}{dt}(\boldsymbol{r} \times m\boldsymbol{v}) = \boldsymbol{r} \times \boldsymbol{F} = 0 \, ,$$

since ***F*** is a central force (***r***//***F***), *L_z is a constant of motion.*

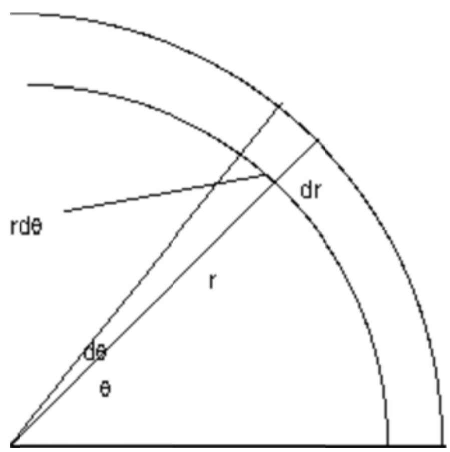
$$l = mrv_\theta = mr^2\dot{\theta}.$$

The velocity v_θ is given by

$$v_\theta = r\dot{\theta} = r\frac{l}{mr^2} = \frac{l}{mr}.$$

A.2 Physical meaning

What is the physical meaning of the constant angular momentum? We now consider the d*A*/dt, where d*A* is the partial area of the ellipse.



$$dA = \frac{1}{2}r^2 d\theta$$

$$\frac{dA}{dt} = \frac{1}{2}r^2\frac{d\theta}{dt} = \frac{1}{2}r^2\dot{\theta} = \frac{l}{2m} = const$$

since $l = mr^2\dot{\theta} = const$. The period *T* is given by

$$T = \int dt = \frac{2m}{l}\int dA = \frac{2m}{l}\pi ab = \frac{2m}{l}\pi a^2\sqrt{1-e^2}$$

since $dt = \frac{2m}{l}dA$.

A.3. The effective potential

The total energy is a sum of the kinetic energy and the potential energy

$$E = \frac{1}{2}mv^2 - \frac{\kappa}{r} = \frac{1}{2}m(v_r{}^2 + v_\theta{}^2) - \frac{\kappa}{r}$$

or

$$E = \frac{1}{2}m(\dot{r}^2 + \frac{l^2}{m^2 r^2}) - \frac{\kappa}{r} = \frac{1}{2}m\dot{r}^2 + \frac{l^2}{2mr^2} - \frac{\kappa}{r}, \qquad (1)$$

The energy is dependent only on r (actually one dimensional problem).

$$U_{eff} = -\frac{\kappa}{r} + \frac{l^2}{2mr^2}. \qquad \text{(effective potential)}$$

The effective potential energy U_{eff} has a local minimum

$$U_{eff}^{\min} = -\frac{m\kappa^2}{2l^2},$$

at

$$r_{\min} = \frac{l^2}{m\kappa} = \frac{p_0}{2}.$$

Since E = constant, we have an equation of motion

$$\frac{dE}{dt} = m\dot{r}\ddot{r} + \frac{\kappa}{r^2}\dot{r} - \frac{l^2}{mr^3}\dot{r}$$
$$= (m\ddot{r} + \frac{\kappa}{r^2} - \frac{l^2}{mr^3})\dot{r} = 0$$

$$m\ddot{r} + \frac{\kappa}{r^2} - \frac{l^2}{mr^3} = 0. \qquad \text{(equivalent 1D problem)}$$

Plot of the effective potential as a function of r

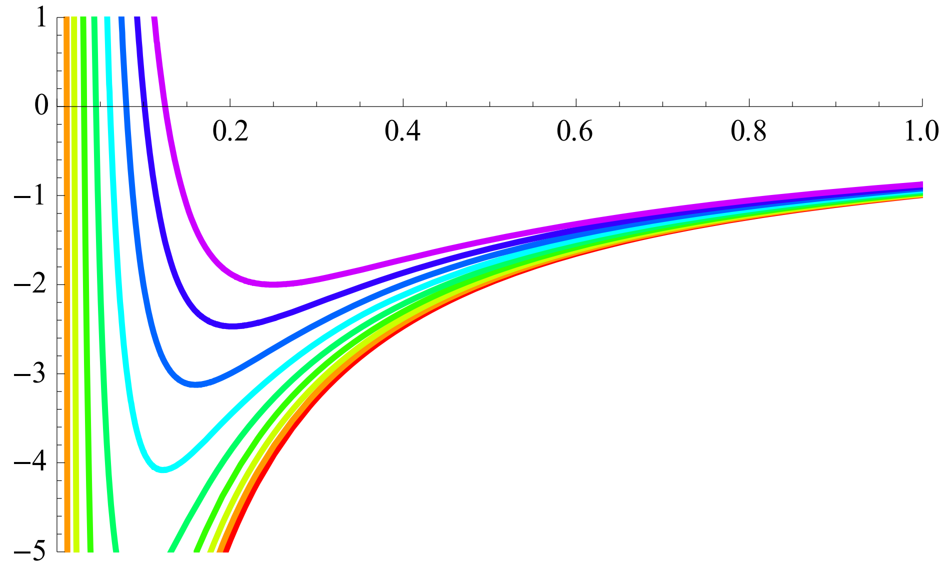


Fig. The effective potential vs r with $l = 0.1 - 0.5$

A.4 Perihelion and aphelion

When $\dot{r} = 0$ for the perihelion (nearest from the Sun) and the aphelion (farthest from Sun) r_1 and r_2 are the roots of Eq.(1).

$$r^2 + \frac{\kappa}{E} r - \frac{l^2}{2mE} = 0 .$$

There are the relations between r_1 and r_2.

$$r_1 + r_2 = -\frac{\kappa}{E} = \frac{\kappa}{|E|} = 2a$$
$$r_1 r_2 = -\frac{l^2}{2mE} = \frac{l^2}{2m|E|}$$

where the total energy is given by

$$|E| = \frac{\kappa}{2a} . \qquad (E<0, \text{ bound state})$$

and

$$r_1 = a(1-e)$$
$$r_2 = a(1+e)$$

From this we have

$$1-e^2 = \frac{r_1 r_2}{a^2} = \frac{l^2}{a^2 2m|E|} = \frac{l^2}{2ma^2}\frac{2a}{\kappa} = \frac{l^2}{m\kappa a}$$

or

p_0 is the semi latus rectum,

$$p_0 = a(1-e^2) = \frac{l^2}{m\kappa}$$

A.5 Kepler's Third Law

$$T = \frac{2m}{l}\pi a^2\sqrt{1-e^2} = \frac{2m}{l}\pi a^2\sqrt{\frac{\ell^2}{m\kappa a}} = \frac{2\pi m a^{3/2}}{\sqrt{m\kappa}},$$

or

$$T^2 = \frac{4\pi^2 m^2 a^3}{m\kappa} = \frac{4\pi^2 m a^3}{\kappa},$$

or

$$\frac{a^3}{T^2} = \frac{\kappa}{4\pi^2 m} = \frac{GmM_{sun}}{4\pi^2 m} = \frac{GM_{sun}}{4\pi^2},$$

or

$$T^2 = \frac{4\pi^2}{GM_{sun}}a^3$$

or

$$[T(year)]^2 = [a(AU)]^3.$$

A.6 Derivation of the Kepler's First Law

We start with

$$m\ddot{r} = mr\dot{\theta}^2 - \frac{\kappa}{r^2}$$

$$mr^2\dot{\theta} = l = constant$$

Here we have

$$ldt = mr^2 d\theta .$$

Note that r depends only on θ.

$$\frac{d}{dt} = \frac{d\theta}{dt}\frac{\partial}{\partial\theta} = \frac{l}{mr^2}\frac{d}{d\theta}$$

$$\frac{d}{dt}(\frac{d}{dt}) = \frac{l}{mr^2}\frac{d}{d\theta}(\frac{l}{mr^2}\frac{d}{d\theta})$$

or

$$\frac{l}{mr^2}\frac{d}{d\theta}(\frac{l}{mr^2}\frac{dr}{d\theta}) = \frac{l^2}{m^2r^3} - \frac{\kappa}{mr^2} .$$

We define u as $u = \frac{1}{r}$,

$$\frac{1}{r^2}\frac{dr}{d\theta} = -\frac{d}{d\theta}(\frac{1}{r}) = -\frac{du}{d\theta} .$$

Then we have

$$\frac{l^2}{m^2r^2}\frac{d}{d\theta}(-\frac{du}{d\theta}) = \frac{l^2}{m^2r^3} - \frac{\kappa}{mr^2} ,$$

or

$$\frac{d^2u}{d\theta^2} + u = \frac{m\kappa}{l^2} .$$

The solution of this equation is given by

$$u = \frac{1}{r} = \frac{m\kappa}{l^2}(1 + C_1 \cos\theta) ,$$

where A is constant, $r_1 = a(1-e)$ for $\theta = 0$, and $r_2 = a(1+e)$ for $\theta = \pi$

$$\frac{1}{r_1} = \frac{m\kappa}{l^2}(1 + C_1) , \qquad \frac{1}{r_2} = \frac{m\kappa}{l^2}(1 - C_1) ,$$

or

$$C_1 = e\frac{\frac{l^2}{m\kappa}}{a(1-e^2)} = e .$$

Then we have

$$r = \frac{p_0}{1 + e\cos\theta} ,$$

with

$$p_0 = a(1-e^2) = \frac{l^2}{m\kappa} .$$