In orbit with the James Webb space telescope

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A 2022 scientific landmark has been the launching of the new *James Webb space telescope* and its journey out to the Lagrange point SE-L2 of the Sun-Earth system (SE-L2 is $\approx 1.5 \cdot 10^6$ km away of Earth). The JWST will not be stationed in L2 exactly, but will follow a periodic 'Halo' orbit around L2, with a 'major' semi-amplitude of order $\approx 0.7 \cdot 10^6$ km and a period near half a year relatively to the Sun-Earth line.

The name *'Halo orbit'* was first used in 1966 by Robert W. Farquhar for a proposed parking orbit around the L2 point of the system Earth-Moon. A communications relay station in this orbit would have in view simultaneously and continuously the Earth and the far side of the Moon.

In 1973 R. Farquhar and A. Kamel *"found that when the in-plane* [i.e.,horizontal] *amplitude of a Lissajous orbit was large enough there would be a corresponding out-of-plane* [i.e.,vertical] *amplitude that would have the same period, so the orbit ceased to be a Lissajous orbit and became approximately an ellipse."* ('Halo orbits' English Wikipedia). These are the actual halo orbits, and this the main idea for the present exercise. Halo orbits exists around L1 and L2 Lagrange points of any system of two primaries, and for the Sun-Earth system have been used since 1978 for several space missions, including ISEE-3 and SOHO in L1 and now JWST in L2. Other missions, as PLANCK, HERSCHEL and GAIA, follow non-periodic Lissajous orbits around L2.

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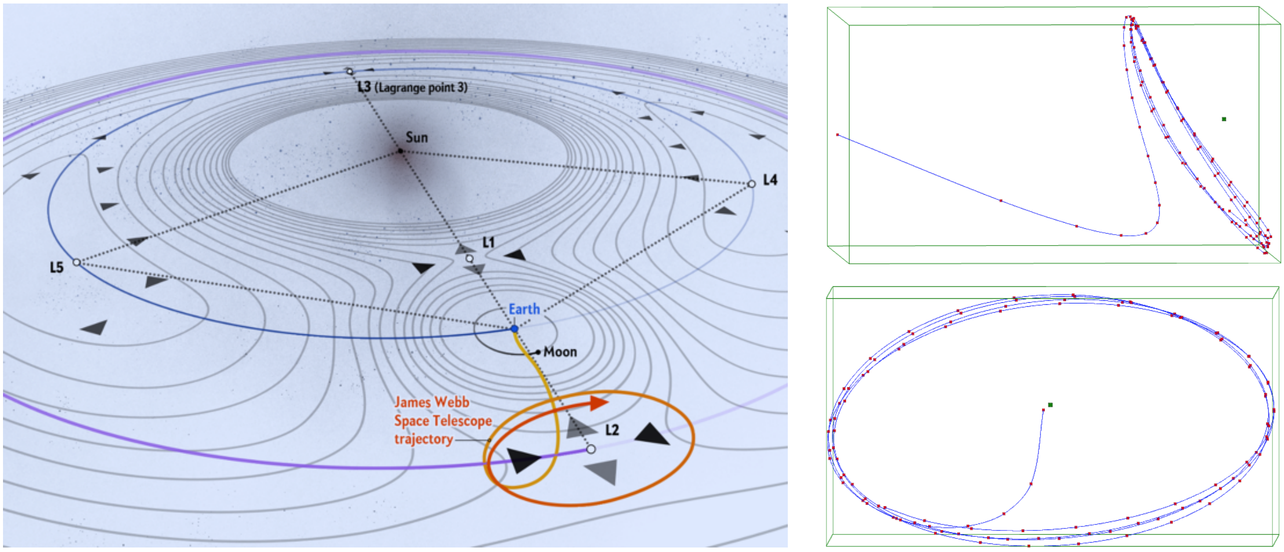
'Never make a calculation until you know the answer', the Wheeler's First Moral Principle says. The exercise should be seen under this light: get a sensible answer before a complete study.

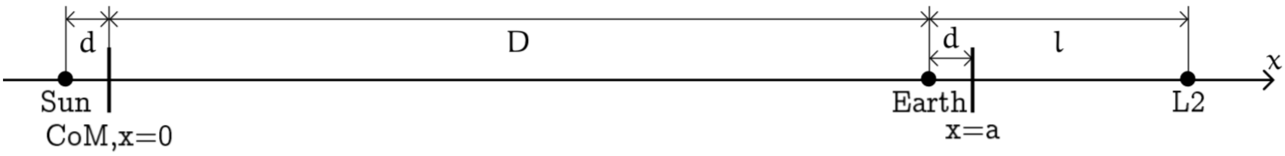


Left: Lagrange points of the Sun-Earth system and the JWST journey out to its halo orbit around L2. (Credit, SciAm). This is not to scale! The group L1-⊕☾-L2 has a local scale greatly exagerated.
Right Reconstructions of the JWST journey and its Halo orbit. The position of L2 is marked in both images. Above, lateral view, Earth at left, Below: view from Sun-Earth line away from L2. (Credit, SageMathCell)

Lets briefly recall on Lagrange points. There are five such points in the system Sun-Earth, all lying in the Earth's orbital plane, and three of them on the Sun-Earth line. Any small object of negligible mass μ as compared to $m \equiv M_\oplus$, $M \equiv M_\odot$, and initially placed at rest relatively to the Sun and Earth in one of these points, will stay there (ignoring any other gravitational effect).

Relatively to a 'barycentric' inertial frame, (origin at the Sun-Earth center of mass), Sun, Earth and the five Lagrange points rotate with the same angular frequency $\Omega = 2\pi\,\text{year}^{-1}$ in the Earth's orbital —ecliptic— plane). In the non-inertial frame which is co-rotating with exactly this angular frequency Ω, the Sun, the Earth and the Lagrange points have fixed positions; this is the frame we will use.

The exercise refers to Lagrange point SE-L2, on the Sun-Earth line (see diagram). You should assume circular orbits for Earth and Sun around the Sun-Earth center of mass and ignore gravitational effects of Moon, Jupiter, etc. In the barycentric inertial frame, L2 follows a circular orbit, of radius larger than that of Earth, but with the same angular frequency Ω than Earth. In the non-inertial co-rotating frame, L2 is at rest; in this frame the total force on a body at this point should vanish.



Along the problem, please use a cartesian coordinate system (x, y, z) *in the co-rotating frame* with origin at the center of mass of the system Sun-Earth, Ecliptic plane (the orbital plane of the Earth) as the xy plane, and Sun and Earth placed on the x axis, at a distance a, with $x_\odot < 0$. Name distances d, D, l along the x axis as per the previous diagram, and call r_1, r_2, r the distances from a general point to the Sun center, to the Earth center and to the z axis (all these distances are taken as positive). Write the Earth mass m as α times the total mass $M+m$ of the system Sun-Earth.

Call $U = U_1 + U_2$ the total *gravitational* potential with U_1, U_2 the ones due to Sun and Earth, V the effective potential (V_{eff}, see B4), and restrict the use of shorthands like U_x, V_{yy}, etc. for the values of the evaluation at L2 of the corresponding x-derivative of U, second yy-derivative of V, etc., avoiding the use of these symbols to denote the derivative functions themselves.

Only the question D7b cannot be approached until D7a has been fully answered. Up to some very basic results, all other questions can be answered independently.

A Basic results on L2 (2 points)

- **A1)** (0.5 points) *List all contributions to the force on a body at rest in L2, i) in the barycentric frame, and ii) in the non-inertial co-rotating frame. In the co-rotating frame, make a sketch (not to scale!) of forces acting on a body at rest in L2.*
- **A2)** (0.5 points) *A small body sitting at L2 —at a distance to the center of mass greater than Earth's— rotates (in the barycentric frame) with the same angular frequency as Earth. How is this possible?*
- **A3)** (1 point) *In an approximation to first order of small quantities, prove that the distance l between Earth and L2 is given by $l \approx a\left(\frac{m}{\beta M}\right)^{1/3}$ where a is the distance Sun-Earth and β is a numerical adimensional coefficient, which should follow from the calculation.*

B Motion of a small body, negligible mass, in the Sun-Earth field (3 points)

Now we consider the possible motions a small body of mass μ negligible relatively to m and M.

- **B4)** (2.75 points, full score for *any correct* derivation) *Using the coordinates described above, prove that the equations of motion of the small body of negligible mass μ have the form (the gravitational field produced by the small body is neglected):*

$$\ddot{x} = -\frac{\partial V_{\text{eff}}}{\partial x} + 2\,\Omega\dot{y}, \qquad \ddot{y} = -\frac{\partial V_{\text{eff}}}{\partial y} - 2\,\Omega\dot{x} \qquad \ddot{z} = -\frac{\partial V_{\text{eff}}}{\partial z} \tag{1}$$

and give the full expression of the effective potential V_{eff} there (hereafter also denoted simply V).

- **B5)** (0.25 points) *These equations have terms linear in the velocities of the small body. To which forces do these terms correspond?*

C Some particular motions transversal to the Ecliptic plane around L2

Motions *transversal* to the plane of the Ecliptic are known as 'vertical' motions, tagging as 'horizontal' the ones contained in the Ecliptic plane. In the *approximated* regime of *very small vertical oscillations* with fixed $x = x_{\text{L2}}$, $y = y_{\text{L2}}$, the point $z = 0$ is an equilibrium point and the z-dependence of the gravitational potential can be approximated by $U(z) \approx U(0) + \frac{1}{2}U_{zz}z^2$, with $U_{zz} := \frac{\partial^2 U}{\partial z^2}\Big|_{L2}$ (notice the centrifugal potential does not depend on z). Enforcing $z(t) = A\sin(\omega_v t)$ to be a periodic solution of the linearized problem $\ddot{z} = -U_{zz}z$ with frequency ω_v leads directly to $\omega_v = \sqrt{U_{zz}}$. The second derivative U_{zz} evaluated at L2 turns out to be $U_{zz} \approx 3.9706\,\Omega^2$ thus leading to the angular frequency of these small oscillations $\omega_v = 1.99263\,\Omega$, corresponding to a period $T_v \approx 2\pi/\omega_v = 1/1.99263\,\text{year} = 0.501848\,\text{year}$, very slightly over half a year. These results are given for use in the next questions.

D Some particular motions in the plane of the Ecliptic around L2 (2.5 points)

Now let us fix attention to 'horizontal' motions which remain exactly in the $z = 0$ plane; actually there are exact solutions of (1) of this type. In the regime of small oscillations, there are two types of such motions; we restrict our attention to *one of these types*, which are periodic, following *ellipses centered at L2, with axes in the SunEarth line and along the perpendicular direction and traversed at a constant angular velocity ω_h.*

- **D6)** (0.5 points) *A body is following one of these motions. Which forces act on it? Make a sketch (not to scale) of these forces. Is the resultant of all forces acting on the body contained exactly/approximately in the Ecliptic plane? And is this resultant exactly/approximately directed to L2? Please choose alternative and comment the reasons of the choices.*
- **D7a)** (1.5 points) *Using only the info on the elliptic form of these orbits given before and the equations of motion (1) linearized around L2, can you find the angular frequency ω_h of these motions? For this question it suffices to give an algebraic equation whose roots will determine this frequency.*
- **D7b)** (0.5 points) *Starting with the algebraic equation just obtained, can you find the value of the frequency ω_h of these 'horizontal motions' as a numerical dimensionless factor times Ω? Tip: In the co-rotating frame the gravitational potential of Sun and Earth has axial symmetry and satisfies Laplace equation. Then use the results stated in C. Hint: The period T_h is a bit above half a year.*

E From motions in the linear approximation to the true Halo orbits (2.5 points)

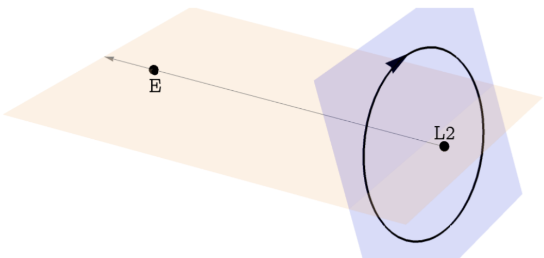
Halo are three-dimensional orbits, which in the co-rotating frame remain 'confined' to a region around L2, and which are *periodic*. The aim of this exercise is to understand how these orbits appear.

As seen before, *in the linear regime of small oscillations* there are confined periodic orbits in the Ecliptic plane, with some frequency ω_h and confined periodic orbits in the 'vertical' direction with angular frequency ω_v. These two frequencies *are not exactly equal, yet they are close*; the data given in C and the calculation in D7 lead in the linear approximation to periods T_h for the horizontal elliptic orbits and T_v for the 'vertical' ones differing only in about 3.5%.

- **E8)** (0.5 points) *Which kind of orbits would arise from superposing an horizontal elliptic orbit and a 'vertical' one, both in the regime of small oscillations? Is this superposition periodic?*

As amplitudes of each of these types of orbits increase, linear approximation is going poorer and poorer. The frequencies of the individual periodic 'horizontal' and 'vertical' motions are expected to change when amplitude increases. Tip: This is what happens with the ordinary pendulum, whose isochrony is only very approximate for very small amplitudes, it isn't?

- **E9)** (1 point) *Elaborate on the clues suggested in the preceding paragraph and explain how it contains the key to make plausible the appearance of tridimensional periodic Halo orbits. In particular, do help the previous explanation to understand i) why these Halo orbits do not exist below some minimum amplitude? and ii) why these orbits were so lately discovered?*



The periodic JWST Halo orbit sits *approximately* on a plane, slanted relatively to the Sun-Earth direction, and its shape in this plane is approximately an ellipse, with center in a point near to L2 on the Sun-Earth line. In the diagram, Earth is the point at the left and L2 the one at right side, both on the thin line Sun-Earth-L2.

- **E10)** (1 point) *Assume a body is following the Halo orbit of the JSWT as given approximately in the diagram. Which are the forces acting on the body, in the co-rotating frame? Sketch them. Is the resultant permanently directed, exactly/loosely, to L2? Why?*

Numerical data
Sun Mass $M_\odot \equiv M \approx 2 \times 10^{30}$ kg. Earth mass $M_\oplus \equiv m \approx 6 \times 10^{24}$ kg.
Angular frequency of the Sun-Earth motion in the barycentric frame $\Omega = 2\pi\,\text{year}^{-1}$.
Other useful data (actually not needed here)
Sun-Earth (mean) distance (AU, astronomical unit) $a_{\odot\oplus} \equiv a \approx 150 \times 10^6$ km
1 year $\approx \pi \times 10^7$s,
Newton gravitational constant: $G \approx 6.67 \times 10^{-11}\,\text{m}^3\text{s}^{-2}\text{kg}^{-1}$

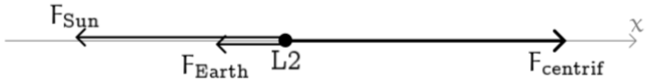
Solution

A Basic results on L2

- **A1)** *List all contributions to the force on a body at rest in L2, i) in the barycentric frame, and ii) in the non-inertial co-rotating frame. In the co-rotating frame, make a sketch (not to scale!) of forces acting on a body at rest in L2.*

i) The gravitational attraction of the Sun and of the Earth, both radial and pointing inwards.

ii) As the frame is not inertial, further to the 'actual' attraction of Sun and Earth, both radial and pointing inwards along the x axis, there are inertial forces. The rotation is uniform and the body is at rest in the frame so there are no Euler nor Coriolis forces. Centrifugal is the only remaining inertial force, which is exactly radial and points outwards with modulus $\mu(D+l)\,\Omega^2$. The resultant is zero.



- **A2)** *A small body sitting at L2 —at a distance to the center of mass greater than Earth's— rotates (in the barycentric frame) with the same angular frequency as Earth. How is this possible?*

For this body to follow a circular orbit with the same angular frequency as Earth's, the inward radial force exerted on it should be larger than the one which the Sun alone would produce at this radial position. Of course, the extra amount of force to make the total force that large is the one provided by the Earth, which in L2 adds to the one produced by the Sun.

- **A3)** *In an approximation to first order of small quantities, prove that the distance l between Earth and L2 is given by $l \approx a\left(\frac{m}{\beta M}\right)^{1/3}$ where a is the distance Sun-Earth and β is a numerical adimensional coefficient, which should follow from the calculation.*

With m written as α times the total Sun-Earth mass, $m = \alpha(M+m)$, then $\alpha \approx 3\cdot 10^{-6}$ and $M = (1-\alpha)(M+m)$. With the suggested notation for distances along the line Sun-Earth, the (positive) distances from the center of mass to the Sun and to Earth centers, d, D are determined by the conditions $d + D = a$ and $Md - mD = 0$, leading to $d = \alpha\, a,\ D = (1-\alpha)\, a$.

The gravitational forces exerted on the small body at L2 by the Sun and the Earth are on the x axis, pointing inwards, and with respective values $-GM\mu/(a+l)^2$ and $-Gm\mu/l^2$. The centrifugal force is outwards, with modulus $\mu(D+l)\,\Omega^2$. The condition determining the position of L2 is:

$$\frac{GM\mu}{(a+l)^2} + \frac{Gm\mu}{l^2} - \mu(D+l)\,\Omega^2 = 0 \tag{2}$$

For the system Sun-Earth, the mutual orbital angular frequency Ω of the system and the distance a between the Sun and the Earth are related by the 123 Kepler law: $G(M+m) = \Omega^2 a^3$, so that $\Omega^2 = \frac{G(M+m)}{a^3}$. If we first replace this expression of Ω^2 in (2), then recall $d = \alpha a$, $D = (1-\alpha)a$ and finally write $l = \lambda a$, where λ is adimensional, we find that G and a disappear and the successive equations determining the position of L2 are

$$\frac{GM}{(a+l)^2} + \frac{Gm}{l^2} - \frac{G(M+m)(D+l)}{a^3} = 0 \quad \Rightarrow \quad \frac{M}{(1+\lambda)^2} + \frac{m}{\lambda^2} - (M+m)(1-\alpha+\lambda) = 0$$

Up to now everything is exact. Make now some approximations. We know $\alpha \approx 3\cdot 10^{-6} \ll 1$, and assume λ is also small in front of 1. Hence terms in $\alpha^2, \alpha\lambda, \lambda^2$ can be neglected against terms linear in α, λ. Thus we can approximate $\frac{M}{(1+\lambda)^2}$ successively by $M(1-\lambda)^2$ and then by $M(1-2\lambda)$. In the last term, to the same order, $(1-\alpha+\lambda)$ can be approximated as $(1-\alpha)(1+\lambda)$. Using $(M+m)(1-\alpha) = M$, the equation reduces to:

$$M(1-2\lambda) + \frac{m}{\lambda^2} - M(1+\lambda) \approx 0 \quad \Rightarrow \quad \frac{m}{\lambda^2} \approx 3M\lambda \;\Rightarrow\; \lambda \approx \left(\frac{m}{3\,M}\right)^{1/3} \quad \Rightarrow \quad l \approx a\left(\frac{m}{3\,M}\right)^{1/3}$$

so the value of β is $\beta = 3$. As the quotient $m/M \approx 3 \cdot 10^{-6}$, the factor $\lambda \approx 10^{-2}$, so the distance $l = \lambda a$ is around one percent of the astronomical unit; as expected, λ is actually small against 1.

Alternatively, should the approximation had been made writing $(a + l)$ instead of $(D + l)$ in (2), then after replacing l by λa we should have arrived directly to $M(1 - 2\lambda) + \frac{m}{\lambda^2} - (M + m)(1 + \lambda) \approx 0$, and neglecting $m(1 + \lambda)$ versus m/λ^2 we would have obtained the same result.

B Motion of a small body, negligible mass, in the Sun-Earth field

- **B4)** *Using the coordinates described above, prove that the equations of motion of the small body of negligible mass μ have the form (the gravitational field produced by the small body is neglected):*

$$\ddot{x} = -\frac{\partial V_{\text{eff}}}{\partial x} + 2\,\Omega\dot{y}, \qquad \ddot{y} = -\frac{\partial V_{\text{eff}}}{\partial y} - 2\,\Omega\dot{x} \qquad \ddot{z} = -\frac{\partial V_{\text{eff}}}{\partial z} \tag{3}$$

and give the full expression of the effective potential V_{eff} there (hereafter also denoted simply V).

The most elementary derivation uses Newtonian mechanics. A more elegant derivation is through Lagrangian formulation.

In the Newtonian way, one needs to know the forces acting on the small body. Within the co-rotating inertial frame, which is rotating with constant angular velocity Ω, further to the gravitational forces due to the Sun and to the Earth on the body, there are inertial forces.

The gravitational force due to the Sun is attractive, directed to the Sun, and at each possible position (x, y, z) of the body its absolute value is $GM\mu/(r_1)^2$, where r_1 is the distance from the point (x, y, z) to the fixed Sun position $(-d, 0, 0)$. This force is well known to be minus the gradient of a potential energy $\mu U_1 = -GM\mu/r_1$, and thus the force components are $\mu\big(-\frac{\partial U_1}{\partial x}, -\frac{\partial U_1}{\partial y}, -\frac{\partial U_1}{\partial z}\big)$. Likewise, the force due to Earth comes as minus the gradient of the potential energy $\mu U_2 = -Gm\mu/r_2$, with components $\mu\big(-\frac{\partial U_2}{\partial x}, -\frac{\partial U_2}{\partial y}, -\frac{\partial U_2}{\partial z}\big)$, where now r_2 is the distance from (x, y, z) to the fixed Earth position $(D, 0, 0)$.

Further to these, there are inertial forces. As the angular velocity of the rotating frame is constant, both in direction and in absolute value, the Euler inertial force which comes from a variable angular velocity is absent. There remain only the centrifugal and Coriolis forces.

The centrifugal force is directed outwards *from the rotation axis*, with absolute value $\mu\, r\, \Omega^2$, where now r is the distance from the actual position of the body (x, y, z) *to the rotation axis*, hence $r = \sqrt{x^2 + y^2}$. The components of this centrifugal force are $\mu\,\Omega^2\,\big(x, y, 0\big)$. Clearly this is also minus the gradient of the so-called *centrifugal potential energy* $\mu\,\Phi = -\frac{1}{2}\mu\, r^2\,\Omega^2 = -\frac{1}{2}\mu\,(x^2 + y^2)\,\Omega^2$.

Finally there are the Coriolis forces, given in the standard vector language as (minus twice) the mass of the body times the vector product of the angular velocity of the frame by the velocity vector of the body in the rotating frame. These vectors are respectively $(0, 0, \Omega)$ and $(\dot{x}, \dot{y}, \dot{z})$, thus leading to $\mu\,(\Omega\dot{y}, -\Omega\dot{x}, 0)$ for the Coriolis force components.

Collecting all terms the Newton equations read (of course μ disappears)

$$\ddot{x} = -\frac{\partial U_1}{\partial x} - \frac{\partial U_2}{\partial x} - \frac{\partial \Phi}{\partial x} + 2\Omega\dot{y}, \qquad \ddot{y} = -\frac{\partial U_1}{\partial y} - \frac{\partial U_2}{\partial y} - \frac{\partial \Phi}{\partial y} - 2\Omega\dot{x} \qquad \ddot{z} = -\frac{\partial U_1}{\partial z} - \frac{\partial U_2}{\partial z}$$

where after dividing by the μ factor in the potential energies, the functions U_1, U_2, Φ are the *true potentials*; the effective potential V_{eff} can be read from these equations and is explicitly given by

$$V_{\text{eff}} = U_1 + U_2 + \Phi, \quad V_{\text{eff}}(x, y, z) = -\frac{GM}{\sqrt{(x+d)^2 + y^2 + z^2}} - \frac{Gm}{\sqrt{(x-D)^2 + y^2 + z^2}} - \tfrac{1}{2}(x^2 + y^2)\Omega^2 \tag{4}$$

Other possible approach is via the Lagrangian formulation. All one needs there is the correct Lagrangian of this system *in the non inertial co-rotating frame.* While one is not supposed to know this beforehand, obtaining it is easy. The starting points are the scalar character of the classical

Lagrangian under any change of coordinates (even depending on time) and the well known form of the Lagrangian in an inertial frame, in presence of forces coming from the external Sun-Earth gravitational potential $U = U_1 + U_2$. Naming X, Y, Z a set of cartesian coordinates in this barycentric inertial frame, the Lagrangian is: $\mathcal{L}(X, Y, Z, \dot{X}, \dot{Y}, \dot{Z}) = \frac{1}{2}\mu\,(\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2) - \mu\,U(X, Y, Z)$.

The gravitational potential is a scalar, so that relatively to the co-rotating frame, the potential $U(x, y, z)$ will simply follow by changing the variables from (X, Y, Z) to (x, y, z) in U. (The distances between any actual position of the small body and the Sun and Earth are geometric quantities, so the potentials, when expressed in terms of r_1, r_2 are the same as in the non-inertial frame, but of course their expressions as functions of the new coordinates will differ).

Now we perform the change of coordinates. Choosing the new Z direction to coincide with the old z, these are given by a simple rotation with angular velocity $-\Omega$ around the z axis:

$$X = x\cos(\Omega t) - y\sin(\Omega t), \qquad Y = x\sin(\Omega t) + y\cos(\Omega t), \quad Z = z$$

Taking the total time derivative in the these expressions and grouping terms, one obtains

$$\dot{X} = (\dot{x} - \Omega y)\cos(\Omega t) - (\dot{y} + \Omega x)\sin(\Omega t), \quad \dot{Y} = (\dot{x} - \Omega y)\sin(\Omega t) + (\dot{y} + \Omega x)\cos(\Omega t), \quad \dot{Z} = \dot{z}$$

A straightforward computation leads to $\dot{X}^2 + \dot{Y}^2 = \big(\dot{x}^2 + \dot{y}^2\big) - 2\Omega\big(\dot{x}y - \dot{y}x\big) + \Omega^2(x^2 + y^2)$.

As the Lagrangian itself should be also a scalar, we get its correct form in the co-rotating frame by simple substitution, which leads to:

$$\mathcal{L}(x, y, z, \dot{x}, \dot{y}, \dot{z}) = \tfrac{1}{2}\mu\,(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \mu\,\Omega\big(\dot{x}\,y - \dot{y}\,x\big) + \tfrac{1}{2}\mu\,\Omega^2(x^2 + y^2) - \mu\,U(x, y, z)$$

where the third term in the r.h.s., being a function only of coordinates, can be incorporated into an *effective potential energy* $\mu\,V_{\text{eff}}(x, y, z) = \mu\,U(x, y, z) - \frac{1}{2}\mu\,\Omega^2\,(x^2 + y^2)$, so the Lagrangian is:

$$\mathcal{L}(x, y, z, \dot{x}, \dot{y}, \dot{z}) = \tfrac{1}{2}\mu\,(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \mu\,\Omega\big(\dot{x}\,y - \dot{y}\,x\big) - \mu\,V_{\text{eff}}(x, y, z)$$

and the three Euler-Lagrange equations of motion are:

$$\left.\begin{array}{l} \dfrac{\partial\mathcal{L}}{\partial\dot{x}} = \mu\,\dot{x} - \mu\,\Omega\,y \;\Rightarrow\; \dfrac{d}{dt}\dfrac{\partial\mathcal{L}}{\partial\dot{x}} = \mu\,(\ddot{x} - \Omega\,\dot{y}) \\ \dfrac{\partial\mathcal{L}}{\partial x} = -\mu\,\dfrac{\partial V_{\text{eff}}}{\partial x} + \mu\,\Omega\,\dot{y} \end{array}\right\} \qquad \ddot{x} - \Omega\,\dot{y} = -\frac{\partial V_{\text{eff}}}{\partial x} + \Omega\,\dot{y}$$

$$\left.\begin{array}{l} \dfrac{\partial\mathcal{L}}{\partial\dot{y}} = \mu\,\dot{y} + \mu\,\Omega\,x \;\Rightarrow\; \dfrac{d}{dt}\dfrac{\partial\mathcal{L}}{\partial\dot{y}} = \mu\,(\ddot{y} + \Omega\,\dot{x}) \\ \dfrac{\partial\mathcal{L}}{\partial y} = -\mu\,\dfrac{\partial V_{\text{eff}}}{\partial y} - \mu\,\Omega\,\dot{x} \end{array}\right\} \qquad \ddot{y} + \Omega\,\dot{x} = -\frac{\partial V_{\text{eff}}}{\partial y} - \Omega\,\dot{x}$$

$$\left.\begin{array}{l} \dfrac{\partial\mathcal{L}}{\partial\dot{z}} = \mu\,\dot{z} \Rightarrow \dfrac{d}{dt}\dfrac{\partial\mathcal{L}}{\partial\dot{z}} = \mu\,\ddot{z} \\ \dfrac{\partial\mathcal{L}}{\partial z} = -\mu\,\dfrac{\partial V_{\text{eff}}}{\partial z} \end{array}\right\} \qquad \ddot{z} = -\frac{\partial V_{\text{eff}}}{\partial z}$$

which are the equations we were looking for. Of course, μ turns out to be irrelevant, and as this should have been clear from the beginning we could/should have taken $\mu = 1$ to start with.

The effective potential is $V_{\text{eff}}(x, y, z) = U(x, y, z) - \frac{1}{2}\Omega^2\,(x^2 + y^2)$ which of course coincides with the one (4) obtained in the newtonian derivation.

- **B5)** *These equations have terms linear in the velocities of the small body. To which forces do these terms correspond?*

  These are the Coriolis forces.

C Some particular motions around L2 transversal to the Ecliptic plane

There was no any question on these motions, but only some final results were given in the formulation. It is worth to discuss how these results can be obtained, referring to the text in C.

- **C)** *Calculate explicitly the derivative appearing in the previous expression of $\omega_v = \sqrt{U_{zz}}$ and transform that expression by using the third Kepler law in the form $G(M+m) = \Omega^2 a^3$ so that the frequency ω_v is finally given by a relation $\omega_v = f_v\,\Omega$ with a dimensionless numerical factor f_v which should be calculated. Hint: The result for the period T_v is a bit below half a year.*

This second z derivative of the gravitational potential can be calculated as follows. First, U is a sum of two potentials created by bodies placed on the x axis. Each such summand has a form $\mathcal{U} = -\frac{G\mathcal{M}}{\rho}$, where $\rho = \sqrt{(x-f)^2 + y^2 + z^2} \equiv (\cdots + z^2)^{1/2}$ is the distance to the source body of mass $\mathcal{M}$. The potential and its first and second z derivatives are:

$$\mathcal{U} = -\frac{G\mathcal{M}}{\sqrt{\cdots + z^2}}, \qquad \frac{\partial \mathcal{U}}{\partial z} = G\mathcal{M}\frac{z}{(\cdots + z^2)^{3/2}}, \qquad \frac{\partial^2 \mathcal{U}}{\partial z^2} = G\mathcal{M}\frac{(\cdots + z^2)^{3/2} - 3\,z^2(\cdots + z^2)^{1/2}}{(\cdots + z^2)^3}$$

which, using the notations $\mathcal{U}_z$, $\mathcal{U}_{zz}$ for the derivatives evaluated at L2, where $x = x_{L2}, y = 0, z = 0$, then $(\cdots + z^2) = (x_{L2} - f)^2 = (\rho|_{L2})^2$ and gives:

$$\mathcal{U}_z := \left.\frac{\partial \mathcal{U}}{\partial z}\right|_{L2} = 0, \qquad \mathcal{U}_{zz} := \left.\frac{\partial^2 \mathcal{U}}{\partial z^2}\right|_{L2} = \frac{G\mathcal{M}}{(x_{L2} - f)^3} = \frac{G\mathcal{M}}{(\rho|_{L2})^3}$$

In our case there are two attracting masses, the Sun, of mass M and at a distance $(a+l)$ from L2, and the Earth, of mass m and at a distance l. Thus for the second z derivative of the total gravitational potential U evaluated at the Lagrange point L2 one has

$$U_{zz} = \frac{GM}{(a+l)^3} + \frac{Gm}{l^3}$$

If now we use $M = (1-\alpha)(M+m)$, $m = \alpha(M+m)$ and $l = \lambda a$, we can factor the common term $\frac{G(M+m)}{a^3}$ which by the 123 Kepler law is equal to Ω^2, so that we finally get an expression of U_{zz} as a multiple of Ω^2, with a dimensionless factor depending on α and λ:

$$U_{zz} = \left\{\frac{1-\alpha}{(1+\lambda)^3} + \frac{\alpha}{\lambda^3}\right\}\Omega^2, \quad \text{which is of the form } U_{zz} = f_v^2\,\Omega^2 \text{ with } f_v^2 = \left\{\frac{1-\alpha}{(1+\lambda)^3} + \frac{\alpha}{\lambda^3}\right\}.$$

As we already know $\alpha = m/(M+m) \approx 3\cdot 10^{-6}$, and $\lambda \approx 10^{-2}$, the numerical value of the adimensional factor in brackets is:

$$f_v^2 = \left\{\frac{1-\alpha}{(1+\lambda)^3} + \frac{\alpha}{\lambda^3}\right\} \approx \frac{1 - 3\cdot 10^{-6}}{(1+10^{-2})^3} + \frac{3\cdot 10^{-6}}{10^{-6}} \approx 4\left(1 - \tfrac{2.94}{4}\cdot 10^{-2}\right) = 3.9706$$

Thus the precise value of U_{zz} and of the frequency ω_v of the small vertical oscillations are

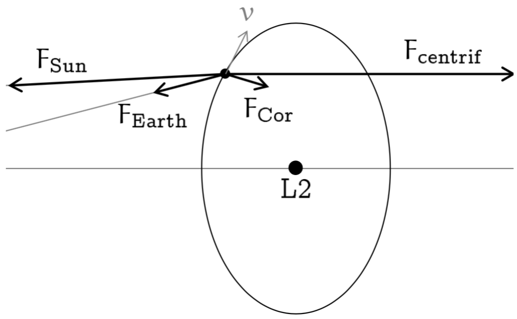
$$U_{zz} \approx 3.9706\,\Omega^2, \qquad \omega_v \approx \sqrt{3.9706}\,\Omega = 1.99263\,\Omega$$

corresponding to a period $T_v = 2\pi/\omega_v \approx 1/1.99263\,\text{year} = 0.501848\,\text{year}$, very slightly over half a year, as said in the C paragraph of the formulation.

D Some particular motions around L2 in the plane of the Ecliptic

- **D6)** *A body is following one of these motions. Which forces act on it? Make a sketch (not to scale) of these forces. Is the resultant of all forces acting on the body contained exactly/approximately in the Ecliptic plane? And is this resultant exactly/approximately directed to L2? Please choose alternative and comment the reasons of the choices.*

Now, to the Sun and Earth attraction and to the centrifugal forces, which are present even when the body is at rest in L2 and which are contained in the xy plane, we should add the Coriolis force, which appears only when the body moves in the non-inertial co-rotating frame. As this force is (minus twice) the vector product of the angular frequency (directed along the z axis) and the velocity vector of the body (contained in the xy plane), this vector product is always contained in the xy plane, which gives again another argument for the existence of solutions with $z = 0$.



Thus, the resultant of all forces is contained exactly in the xy plane (otherwise the z component of the motion could not be $z(t) = 0$). But as these orbits are not circles traversed at a uniform speed, one should not expect this resultant to point exactly to L2.

- **D7a)** *Using only the info on the elliptic form of these orbits given before and the equations of motion (1) linearized around L2, can you find the angular frequency ω_h of these motions? For this question it suffices to give an algebraic equation whose roots will determine this frequency.*

As the statement says that the orbit should be an ellipse around L2, with one axis in the Sun-Earth direction, and traversed with constant angular velocity, we should try with an ansatz:

$$x(t) = x_{L2} + A\,\cos(\omega t), \quad y(t) = y_{L2} + B\,\sin(\omega t), \quad z(t) = 0 \tag{5}$$

with unknown quantities A, B, ω, where here ω stands for ω_h. But this should be a solution of the (linearized) equations of motion, where potentials are approximated up to second order terms, $V \approx V|_{L2} + \frac{1}{2}V_{xx}(x - x_{L2})^2 + \frac{1}{2}V_{yy}(y - y_{L2})^2$, (recall $V_{xx} := \frac{\partial^2 V_{\text{eff}}}{\partial x^2}\Big|_{\text{L2}}$, etc.)

The velocities and accelerations along this motion are

$$\begin{aligned} \dot{x}(t) &= -A\,\omega\sin(\omega t), \qquad & \ddot{x}(t) &= -A\,\omega^2\cos(\omega t) \\ \dot{y}(t) &= \;\;\, B\,\omega\cos(\omega t), \qquad & \ddot{y}(t) &= -B\,\omega^2\sin(\omega t) \end{aligned}$$

Enforcing (5) to be actually a solution of the linearized equations of motion and grouping terms:

$$\cos(\omega t)\left\{\left(\omega^2 - V_{xx}\right)A + \left(2\Omega\omega\right)B\right\} + \sin(\omega t)\left\{V_{xy}B\right\} = 0$$

$$\cos(\omega t)\left\{-V_{xy}A\right\} + \sin(\omega t)\left\{\left(2\,\Omega\,\omega\right)A + \left(\omega^2 - V_{yy}\right)B\right\} = 0$$

Now, as the functions $\cos(\omega t)$ and $\cos(\omega t)$ are linearly independent, all the groups in brackets should vanish. Were the crossed second derivatives $V_{xy} \equiv \frac{\partial^2 V_{\text{eff}}}{\partial x \partial y}\Big|_{\text{L2}}$ different from 0, this would imply $A = B = 0$, and this solution, staying at L2 forever, should not be considered periodic. Hence, (5) could only be a *truly periodic* solution if $V_{xy} = 0$. Of course, this is what occurs because the ellipse axes are exactly in the principal directions of the matrix of the second derivatives of the potential at L2, which is a consequence of the symmetry indicated in the problem formulation.

Hence the conditions ensuring (5) is a solution are:

$$\left(\omega^2 - V_{xx}\right)A + \left(2\,\Omega\,\omega\right)B = 0$$

$$\left(2\,\Omega\,\omega\right)A + \left(\omega^2 - V_{yy}\right)B = 0$$

which is simply a linear system for A, B. There is a non-trivial solution for A, B if the determinant of the matrix of coefficients vanish. This condition, when expanded:

$$\begin{vmatrix} \omega^2 - V_{xx} & 2\Omega\omega \\ 2\Omega\omega & \omega^2 - V_{yy} \end{vmatrix} = 0 \qquad \Rightarrow \qquad \left(\omega^2 - V_{xx}\right)\left(\omega^2 - V_{yy}\right) - 4\Omega^2\omega^2 = 0$$

leads to a biquadratic equation, whose roots determine the frequency ω. Setting $\Lambda := \omega^2$, Λ should satisfy a quadratic equation

$$\Lambda^2 - \big(4\Omega^2 + V_{xx} + V_{yy}\big)\Lambda + V_{xx}V_{yy} = 0$$

The knowledgeable reader will have noticed that this approach is an example of *'speaking prose without realising it'*, as Mr. Jourdain did. The prose here is the general theory of linearisation of a dynamical system around a critical point.

- **D7b)** *Starting with the algebraic equation just obtained, can you find the value of the frequency ω_h of these 'horizontal motions' as a numerical dimensionless factor times Ω? Tip: In the co-rotating frame the gravitational potential of Sun and Earth has axial symmetry and satisfies Laplace equation. Then use the results stated in C. Hint: The period T_h is a bit above half a year.*

  The two roots of the previous equation are

$$\Lambda = \tfrac{1}{2}\Big((4\Omega^2 + V_{xx} + V_{yy}) \pm \sqrt{(4\Omega^2 + V_{xx} + V_{yy})^2 - 4V_{xx}V_{yy}}\Big) \tag{6}$$

(but as $\omega = \sqrt{\Lambda}$, only the positive roots for Λ will be relevant here). For the second derivatives of $V \equiv V_{\text{eff}}$ evaluated at L2, we have

$$V_{xx} = U_{xx} - \Omega^2, \qquad V_{yy} = U_{yy} - \Omega^2$$

(U_{xx}, U_{yy} are the quantities analogous to V_{xx}, V_{yy} but referred to the purely gravitational potential). There is no need (!) of blindly calculating these second derivatives, as there are some general relations which using the results in C allow bypassing the calculations completely (nevertheless, if wanted, these computations can be made ab initio). The second x derivative of the gravitational potential can be calculated as follows. First, as outside the two attracting bodies U is a solution of the Laplace equation, at L2 we should have

$$U_{xx} + U_{yy} + U_{zz} = 0 \qquad \Rightarrow \qquad U_{xx} = -U_{yy} - U_{zz}$$

Furthermore, the gravitational potential U has (in the co-rotating frame) axial symmetry around the x axis, so that we should have as well

$$U_{yy} = U_{zz} \qquad \Rightarrow \qquad U_{xx} = -2\,U_{zz}$$

These relations lead finally to

$$V_{xx} = -2\,U_{zz} - \Omega^2, \qquad U_{yy} = U_{zz} - \Omega^2$$

As previously we mentioned in C that $U_{zz} \approx 3.9706\,\Omega^2$, we get directly

$$V_{xx} \approx -8.9412\,\Omega^2, \qquad V_{yy} \approx 2.9706\,\Omega^2$$

and by replacing in (6) above we get the two roots

$$\Lambda \approx \begin{cases} 4.26174\,\Omega^2 & \Rightarrow \quad \omega_h = \omega \approx 2.0644\,\Omega \\ -6.23233\,\Omega^2 & \Rightarrow \quad \text{as } \Lambda < 0 \text{, this is not an acceptable root here} \end{cases}$$

Hence, the angular frequency of the horizontal elliptic trajectories around L2 in the Ecliptic plane is $\omega_h \approx 2.0644\,\Omega$, which corresponds to a period $T_h \approx 0.48440$ year, slightly under half a year.

Marginal note: The pure imaginary value $\pm\sqrt{-6.23233}\,\Omega = \pm 2.4964\,\mathrm{i}\,\Omega$ which would follow for the *frequency* ω_h from the discarded root correspond to the other 'small oscillation' mode near L2 with motion along proper outgoing and ingoing eigendirections given by a time dependence $e^{\pm 2.4964\,t}$; in dynamical systems lenguaje this is a saddle, making the point L2 globally unstable.

E From motions in the linear approximation to the true Halo orbits

- **E8)** *Which kind of orbits would arise from superposing an horizontal elliptic orbit and a 'vertical' one, both in the regime of small oscillations? Is this superposition periodic?*

As the two angular frequencies are slightly different, these superpositions, called Lissajous orbits, will not be 'simply' periodic, i.e., with horizontal and vertical motions completing a full period in the same time.

- **E9)** *Elaborate on the clues suggested in the preceding paragraph and explain how it contains the key to make plausible the appearance of tridimensional periodic Halo orbits. In particular, do help the previous explanation to understand i) why these Halo orbits do not exist below some minimum amplitude? and ii) why these orbits were so lately discovered?*

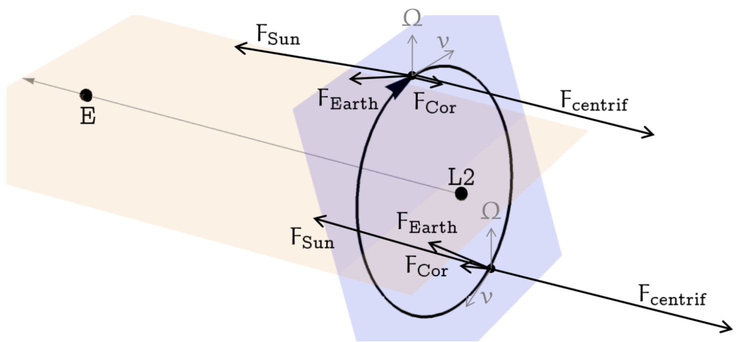
If at the small oscillations level the two frequencies are nearby, and if they are expected to change when the amplitudes increase, it is possible that once the amplitude of horizontal orbits increases enough, its angular frequency will coincide with the angular frequency of a suitable 'vertical mate' (also of not small amplitude). Should this happen, the corresponding common period will likely be some value near to both $T_h = 0.4844$ year and $T_v = 0.5018$ year, this is, near half a year, as mentioned in the introduction. If we were in the linear superposition regime this would mean directly a periodic superposition. Even far from this linear regime, when the involved superposition *is not linear*, this reasoning suggests —albeit only heuristically—, the existence of these expected periodic orbits.

i) These require a minimum amplitude because in the limit of small amplitudes (small oscillations) their angular frequencies are *not equal*, so these periodic three-dimensional orbits cannot exist in the (linear) small oscillations regime.

ii) They were not easy to discover; as they have a essentially non-linear character, they cannot be discovered while using only linear tools.

- **E10)** *Assume a body is following the Halo orbit of the JSWT as given approximately in the diagram. Which are the forces acting on the body, in the co-rotating frame? Sketch them. Is the resultant permanently directed, exactly/loosely, to L2? Why?*

In addition to the gravitational pulls of Sun and Earth and the centrifugal force, which would cancel exactly at L2, and which acts also at any point of the Halo orbit (though with a non-zero partial resultant), as the body is moving with a velocity $\mathbf{v}$ tangent to the trajectory at each point, there is an extra Coriolis force perpendicular to $\mathbf{\Omega}$ and to $\mathbf{v}$ which is represented also in the sketch.



The global resultant should point always grosso modo to the Sun-Earth-L2 line (as the orbit is around this line), but as the halo orbit is not a circle traversed at constant velocity, this force will not point exactly to any fixed location. However, the diagram makes it clear that the global resultant is always directed 'inwards'. While we are used to orbits similar to these when the dominant force is the attraction of a large body placed at its center, here the absence of any 'attracting mass at the center' make these orbits a bit puzzling at the first sight. This apparently puzzling character is disentangled when we realize that the net force, always directed inwards, is actually the resultant of the gravitational attractions of Sun and Earth, the centrifugal force and the Coriolis force.

The stability of the Levitron$^{\text{TM}}$

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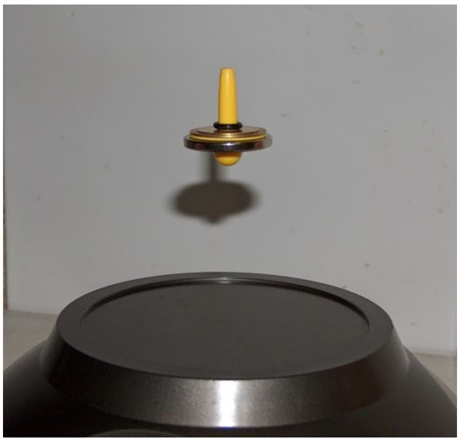

"Levitron™" is a magnetic toy consisting of a spinning top hovering above a base formed by a block of magnetized material. The top is made of a magnetic ceramic and stays in the air due to the repulsion of the powerful magnet at the base, since the equal poles of the magnet and the base are facing each other.
The set consists of a magnetized top, a thin (lifting) plastic plate, and a magnetized square base plate (base). To operate the top, one should set it spinning on the plastic plate that covers the base. The plastic plate is then raised slowly with the top until a point is reached in which the top leaves the plate and continues to spin in midair above the base for a few minutes.

The spin of the top has the function of keeping it oriented in such a way that the magnetic poles of the top and the base repel each other. Without rotation the top overturns, subjected to the couple of forces of the magnetic field of the base, and falls attracted by it. For the top to float freely, it is necessary that its weight and turning speed are finely tuned. In this problem we are going to study the conditions under which the levitron maintains stable levitation.

1. Expansion of the magnetic field around the levitation point (1 point)

The magnetic field that levitates the spinning top is the one created by the base. Set the origin of the coordinates at the point where the levitron floats in equilibrium. There are no field sources at this point. Therefore, the following equations are satisfied:

$$\nabla \cdot \mathbf{B} = 0 \quad \text{and} \quad \nabla \times \mathbf{B} = 0 \tag{1}$$

Assuming that the field created by the base has symmetry of revolution around the z axis, show that the field in the neighborhood of the equilibrium point can be expressed as:

$$B_z = B_0 + Sz + Kz^2 - \frac{1}{2}Kr^2 \tag{2}$$

$$B_r = -\frac{1}{2}Sr - Krz \tag{3}$$

where (r, φ, z) are cylindrical coordinates whose origin is the equilibrium point and B_0, S, and K are constants.

2. Equilibrium condition in the vertical direction (1 point)

The top is a rotationally symmetric body with mass m whose center of mass is located at $\mathbf{r}$. Due to rotation, it has an angular momentum relative to the center of mass $\mathbf{S}$. In addition, it can be regarded as a magnetic dipole with a fixed magnetic moment $\boldsymbol{\mu}$ of magnitude μ located at the center of mass $\mathbf{r}$ and directed along the axis of symmetry of the top. The gradients of the magnetic field compensate for the weight of the top, providing a repulsive force that acts on $\boldsymbol{\mu}$. The top would overturn and fall if it weren't for the gyroscopic effect of $\mathbf{B}$ on $\mathbf{S}$ that provides the mechanism for the top to spin stably above the base.

The total force on the dipole is:

$$\mathbf{F} = -mg\mathbf{e}_z + \nabla(\boldsymbol{\mu} \cdot \mathbf{B}) \tag{4}$$

where $\mathbf{B}$ is the magnetic field due to the base and $\mathbf{e}_z$ the unit vector in the z direction.

Since the field decreases in absolute value as we move away from the base, the equilibrium condition can only be satisfied if the field and the dipole moment $\boldsymbol{\mu}$ point in the opposite direction. Only in that case does the base repel the spinning top.

Express the equilibrium condition in the z direction in terms of the parameters that model the magnetic field: B_0, S and K.

3. Earnshaw's theorem (1 point)

The equilibrium condition in the z direction does not ensure that the spinning top is in stable equilibrium. In fact, Earnshaw's theorem ensures that a stable mechanical equilibrium cannot be achieved only by electrostatic or magnetostatic forces.

Show that regardless of the alignment of the top, any possible equilibrium point is a saddle point. That is, if the equilibrium position is stable on the z axis is unstable transversely, and vice versa.

4. Approximate top rotations (1 point)

As written above, to operate the Levitron one should set the top spinning on the plastic plate that covers the base. In addition, the magnetic field exerts a torque $\boldsymbol{\mu} \times \mathbf{B}$ on the top in such a way that:

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\mu} \times \mathbf{B} \tag{5}$$

where $\mathbf{S}$ is the angular momentum of the top relative to the center of mass.

Experience shows that for the top to lift one has to put it spinning very fast on the plastic plate. In these conditions, the top angular momentum $\mathbf{S}$ can be considered parallel to its angular velocity vector and its symmetry axis, so its initial angular momentum is $\mathbf{S} = I_3\boldsymbol{\omega}$, where I_3 and $\boldsymbol{\omega}$ are the moment of inertia and angular velocity about its symmetry axis. Besides, the magnetic moment is parallel to the symmetry axis.

Transform Eq. (5) for the angular momentum into an equation for the magnetic moment.

In the regime where Levitron works, the top precession is faster than the center-of-mass motion. In these conditions we can consider $(x(t), y(t), z(t))$, and so $\mathbf{B}(t)$, as constant in the time interval while the top is precessing an angle 2π.

Solve the motion of the magnetic moment, Eq. (5), with $\mathbf{B}$ frozen. To do this, call $\mathbf{e}_z$ the direction of $\mathbf{B}$ and consider an arbitrarily oriented dipole[1]

$$\boldsymbol{\mu} = -(\mu_x(t)\ \mathbf{e}_x + \mu_y(t)\ \mathbf{e}_y + \mu_z(t)\ \mathbf{e}_z), \quad \mathbf{B} = B\ \mathbf{e}_z, \ \text{ where } B = |\mathbf{B}(x,y,z)| \text{ and } \mu = |\boldsymbol{\mu}(t)|, \tag{6}$$

Make a sketch showing the motion of the top. Identify the quantities that remain constant during the motion.

5. Stable equilibrium condition (1 point)

The key for the levitron to work is that the top precesses around the local direction of the field, maintaining, on average, the projection of the dipole moment onto the direction of the field. In the fast precession regime of the top, where the magnetic field can be considered frozen during the course of a period $T = 2\pi/\Omega$, the product $\boldsymbol{\mu}(t) \cdot \mathbf{B}(t)$ can be approximated by its average:

$$\overline{\boldsymbol{\mu}(t) \cdot \mathbf{B}(t)} = \frac{1}{T}\int_0^T dt\, \boldsymbol{\mu}(t) \cdot \mathbf{B} \tag{7}$$

[1] The minus sign ensures that $\boldsymbol{\mu}$ and $\mathbf{B}$ are antiparallel when aligned.

Calculate $\overline{\boldsymbol{\mu}(t)\cdot\mathbf{B}(t)}$.

Assume that the energy of the top can be approximated by

$$U \simeq mgz - \overline{\boldsymbol{\mu}\cdot\mathbf{B}} = mgz + \mu_B B \tag{8}$$

with μ_B a constant.

Determine the new equilibrium conditions. Show that stable equilibrium is possible and give the conditions for it to hold.

Section 6. Equations of motion in the linear approximation (2 points)

The top motion is described by the three Cartesian coordinates of the center of mass (x, y, z) and three angles that determine the orientation of the top. Instead of the standard Euler angles, we will use the angles in the convention referred to as xyz[2]. In this convention, the orientation of the spinning top in space is determined by three angles: ψ, θ and ϕ. The angle ψ represents a rotation around the z axis. For an object with axial symmetry, such as the spinning top, it denotes a rotation of the object around its axis of symmetry. The angle θ is a rotation about the y axis. The third angle, ϕ, is a rotation about the x axis. The figures Fig.1 to Fig. 4 illustrate the three successive rotations.

The angular velocity of the top has the values $\dot\theta$ and $\cos\theta\dot\phi$ along the two axes perpendicular to the axis of symmetry, and the value $\dot\psi + \sin\theta\dot\phi$ along the axis of symmetry. The Lagrangian function is (we neglect air friction):

$$\mathcal{L}(x, y, z, \psi, \theta, \phi) = \frac{1}{2}m(\dot x^2 + \dot y^2 + \dot z^2) + \frac{1}{2}I_1(\dot\theta^2 + \cos^2\theta\dot\phi^2) + \frac{1}{2}I_3(\dot\psi + \sin\theta\dot\phi)^2 - U(x, y, z, \psi, \theta, \phi) \tag{9}$$

where m is the mass of the spinning top, I_3 the moment of inertia about the axis of symmetry, and I_1 the moment of inertia about an axis perpendicular to the axis of symmetry.

The axis of the spinning top is oriented along the vector $\mathbf{n} = \sin\theta\mathbf{e}_x + \cos\theta\sin\phi\mathbf{e}_y + \cos\theta\cos\phi\mathbf{e}_z$, and the potential energy is:

$$U = mgz + \mu(B_x\sin\theta + B_y\cos\theta\sin\phi + B_z\cos\theta\cos\phi) \tag{10}$$

The equations of motion have an exact solution when the top spins with constant velocity, at the equilibrium point, and vertically oriented. That is:

$$x = 0,\ y = 0,\ z = 0,\ \phi = 0,\ \theta = 0,\ \psi = \omega t, \tag{11}$$

where ω is the spinning angular velocity.

The equations of motion corresponding to the above Lagrangian constitute a set of nonlinear ordinary differential equations. Because of this non-linear character, an analytical solution of the complete set for any initial conditions is not possible, in general. However, some important features of the levitron dynamics may be obtained from the linear approximation of these equations.

To obtain the linear equations, we can proceed in two ways. A first procedure consists in linearizing the corresponding Euler-Lagrange equations to the Lagrangian obtained above. The second procedure, which is the one we recommend, consists in expanding the Lagrangian retaining the quadratic terms in the perturbations and obtaining, from there, the equations of motion.

Taking all of the above into account, show that the equations of motion of the spinning top in the linear approximation are:

[2] These angles are known in aeronautics as yaw, pitch, and roll.

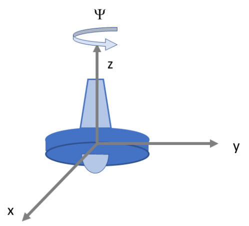

Fig.1 Angle ψ: rotation around OZ.

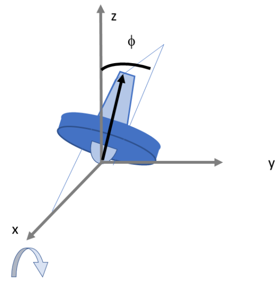

Fig. 3 Angle ϕ: rotation around OX.

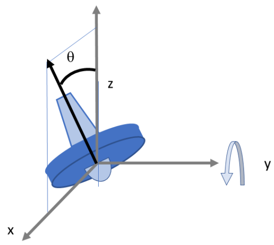

Fig.2 Angle θ: rotation around OY.

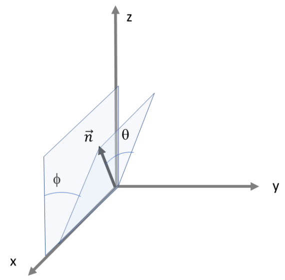

Fig. 4 Vector **n** and its corresponding angles.

$$m\ddot{x} = \frac{1}{2}\mu S\theta + \mu K x \qquad (12a) \qquad I_1\ddot{\theta} = I_3\omega\dot{\phi} + \frac{1}{2}\mu S x + \mu B_0\theta \qquad (12d)$$

$$m\ddot{y} = \frac{1}{2}\mu S\phi + \mu K y \qquad (12b) \qquad I_1\ddot{\phi} = -I_3\omega\dot{\theta} + \frac{1}{2}\mu S y + \mu B_0\phi \qquad (12e)$$

$$m\ddot{z} = -2\mu K z \qquad (12c) \qquad I_3\delta\ddot{\psi} = 0 \qquad (12f)$$

(Note: except for the variable ψ, the disturbances and the unknowns are the same, for example, $\delta x = x$.)

7. Solutions in simple cases (1 point)

1.- The vertical motion equation (z axis) is uncoupled and corresponds to a harmonic oscillator. Find the frequency of the corresponding vertical oscillations (this oscillatory motion is quite visible in practice).

2.- Analyze the solutions in the absence of a magnetic field. This corresponds to the precession of a free top.

3.- Assume a constant magnetic field. This case is analogous to the spin precession around a magnetic field (Larmor precession). Find the solution of the above set of differential equations neglecting the inertial terms (the second derivative of the unknowns).[3]

8. Dispersion relation and lower limit of rotational speed (2 points)

The set of equations (12a-12f) governs the evolution of the perturbations of (11). The levitron will hover stably if these perturbations do not grow exponentially in time.

Propose solutions of the form $e^{i\alpha t}$ for the four unknowns x, y, θ, and ϕ, and find the equation that must satisfy α (dispersion relation). This equation provides α as a function of ω. The range of values of ω for which α is real determines the limits of the rotation speed that allow a stable flight.

[3] The calculations in **7** and **8** become easier using the variables $u = x + iy$ and $v = \theta + i\phi$.

The resulting equation is of fourth order and must be solved graphically or numerically. However, the lower limit of the speed of rotation corresponds to a uniform field and can be found analytically.

Set $S = 0$ and $K = 0$ in the dispersion relation and find the minimum value of ω for α to be real.

Solutions

Section 1. Expansion of the magnetic field around the levitation point

Expanding B_z up to terms of order 2 we have:

$$B_z = B_0 + Sz + Kz^2 + Mr^2 + \dots \tag{13}$$

From the curl of B we obtain:

$$\frac{\partial B_r}{\partial z} = \frac{\partial B_z}{\partial r} = 2Mr \tag{14}$$

integrating:

$$B_r = 2Mrz + Lr + Nr^2 + \dots \tag{15}$$

We now apply the null divergence condition:

$$\frac{1}{r}\frac{\partial (rB_r)}{\partial r} + \frac{\partial B_z}{\partial z} = 0 \tag{16}$$

which yields:

$$4Mz + 2L + 3Nr = -S - 2Kz \tag{17}$$

Identifying the coefficients of z, r, and the independent term, the result is obtained.

Section 2. Equilibrium condition in the vertical direction

The force is:

$$F_z = -mg - \mu\frac{\partial B_z}{\partial z} \tag{18}$$

using the expression for the magnetic field obtained in the previous section:

$$F_z = -mg - \mu(S + 2Kz) \tag{19}$$

taking the equilibrium point as the origin of coordinates:

$$\mu S + mg = 0 \tag{20}$$

That the value of S is negative indicates that the field must be decreasing.

Section 3. Earnshaw's theorem

The energy of the top is

$$U = mgz - \boldsymbol{\mu}\cdot\mathbf{B} \tag{21}$$

With the dipole oriented antiparallel near $r = 0$ and $z = 0$, we have:

$$U = mgz + \mu_z(B_0 + Sz + Kz^2 - \frac{1}{2}Kr^2) + \mu_r(\frac{1}{2}Sr + Krz) \tag{22}$$

The equilibrium conditions are:

$$U_z = 0 \quad \text{and} \quad U_r = 0 \tag{23}$$

that gives:

$$mg + \mu S = 0 \quad \text{and} \quad \mu_r = 0 \tag{24}$$

where we have taking into account that $z = 0$ corresponds to the equilibrium point. This leads to

$$U_{zz} = 2\mu K,\ \ U_{rr} = -\mu K,\ \ U_{zr} = U_{rz} = \mu_r K = 0,\quad \begin{vmatrix} U_{zz} & U_{zr} \\ U_{zr} & U_{rr} \end{vmatrix} = -2(\mu K)^2 < 0 \tag{25}$$

Regardless of the values of the parameters involved, we have a saddle point. Therefore, there is no stable equilibrium point. This is a direct consequence of the fact that B_z satisfies the Laplace equation.

Section 4. Approximate top rotations

Here we make the assumption that the top is fast, in the sense that its angular momentum can be regarded as parallel to both its angular velocity vector and the symmetry axis .

With the simplifying assumption that $\mathbf{S}$ is aligned with the axis of symmetry of the top, $\mathbf{S} = (I_3\omega/\mu)\boldsymbol{\mu}$, we can write

$$\dot{\mathbf{S}} = \frac{\mu}{I_3\omega}\mathbf{S}\times\mathbf{B} \quad \text{or, alternatively} \quad \dot{\boldsymbol{\mu}} = \frac{\mu}{I_3\omega}\boldsymbol{\mu}\times\mathbf{B}. \tag{26}$$

The equation of motion for a freely spinning top precessing with angular velocity $\boldsymbol{\Omega}$ is:

$$\dot{\mathbf{S}} = \boldsymbol{\Omega}\times\mathbf{S} \tag{27}$$

Comparing this with Eq.(26) we conclude that

$$\boldsymbol{\Omega} = -\frac{\mu}{I_3\omega}\mathbf{B} \tag{28}$$

Finally, while the top rotates around its symmetry axis with angular velocity $\omega\mathbf{e}$, it is precessing around $\mathbf{B}$ with angular velocity $\Omega = -\frac{\mu B}{I_3\omega}$. That the angular momentum of the top $\mathbf{S}$ is parallel to the angular velocity and to the axis of the top is untenable unless the angular velocity along the symmetry axis is much larger than precession angular velocity, $\omega \gg |\Omega|$.

On the other hand, in the regime where Levitron works, Ω is so large that the top precession is faster than the center of mass motion. In these conditions we can consider $(x(t), y(t), z(t))$, and so $\mathbf{B}(t)$, as constant in the time interval while the top is precessing 2π.

We will solve the motion of the magnetic moment, Eq. (26), with $\mathbf{B}$ frozen. To do this, call $\mathbf{e}_z$ the direction of $\mathbf{B}$ and consider an arbitrarily oriented dipole[4]

$$\boldsymbol{\mu} = -(\mu_x(t)\ \mathbf{e}_x + \mu_y(t)\ \mathbf{e}_y + \mu_z(t)\ \mathbf{e}_z), \quad \mathbf{B} = B\ \mathbf{e}_z, \ \text{ where } B = |\mathbf{B}(x,y,z)| \text{ and } \mu = |\boldsymbol{\mu}(t)|, \tag{29}$$

Plugging these into Eq. (26) gives

$$\dot{\mu_x} = \Omega\mu_y \tag{30}$$
$$\dot{\mu_y} = -\Omega\mu_x \tag{31}$$
$$\dot{\mu_z} = 0 \tag{32}$$

which gives

$$\boldsymbol{\mu} = -(\mu_\perp\cos(\Omega t+\beta)\ \mathbf{e}_x - \mu_\perp\sin(\Omega t+\beta)\ \mathbf{e}_y + \mu_\parallel\ \mathbf{e}_z), \quad \mathbf{B} = B\ \mathbf{e}_z \tag{33}$$

where the phase β is determined by the initial conditions. The angle γ between $\boldsymbol{\mu}$ and $\mathbf{B}$ remains constant, so $\mu_\parallel = \mu\cos\gamma$ and $\mu_\perp = \mu\sin\gamma$.

Section 5. Stable equilibrium condition

In the fast precession regime of the top, where the magnetic field can be considered frozen during the course of a period $T = 2\pi/\Omega$, the product $\boldsymbol{\mu}\cdot\mathbf{B}$ can be substituted by its average:

$$\overline{\boldsymbol{\mu}(t)\cdot\mathbf{B}(t)} = \frac{1}{T}\int_0^T dt\boldsymbol{\mu}(t)\cdot\mathbf{B} = -\frac{1}{T}\int_0^T dt\mu\cos\gamma\ B = -\mu\cos\gamma\ B = -\mu_B B, \tag{34}$$

i. e., a constant, μ_B, times the absolute value of the field.

[4] The minus sign ensures that $\boldsymbol{\mu}$ and $\mathbf{B}$ are antiparallel when aligned.

In this case, the energy of the top is:

$$U \simeq mgz - \overline{\boldsymbol{\mu}(t) \cdot \mathbf{B}(t)} = mgz + \mu_B \sqrt{B_r^2 + B_z^2} \tag{35}$$

To study the equilibrium, it is enough to expand B to second order in r and z

$$\begin{aligned} \sqrt{B_r^2 + B_z^2} &= \sqrt{B_0^2 + 2B_0 S z + (2B_0 K + S^2) z^2 + \left(\frac{S^2}{4} - K B_0\right) r^2} \qquad (36) \\ &= B_0 \left\{ 1 + \frac{S}{B_0} z + \frac{1}{2} \left(\frac{2K}{B_0} + \left(\frac{S}{B_0}\right)^2 \right) z^2 + \left(\left(\frac{S}{2B_0}\right)^2 - \frac{K}{B_0} \right) r^2 - \frac{1}{8} \left(\frac{2S}{B_0}\right)^2 z^2 \right\} \end{aligned}$$

where the last term in z^2 comes from $(1+x)^{1/2} = 1 + x/2 - x^2/8 + \ldots$. The equilibrium conditions are now

$$mg + \mu_B \frac{\partial B}{\partial z} = mg + \mu_B (S + 2Kz) = 0 \text{ with } z = 0 \Rightarrow \; mg + S = 0 \tag{37}$$

$$\mu_B \frac{\partial B}{\partial r} = \mu_B \left(\left(\frac{S}{2B_0}\right)^2 - \frac{K}{B_0} \right) r = 0 \Rightarrow r = 0 \tag{38}$$

The condition that U is a minimum at $z = 0$ requires

$$\mu_B \frac{\partial^2 B}{\partial z^2} = 2\mu_B K > 0 \tag{39}$$

$$\mu_B \frac{\partial^2 B}{\partial r^2} = \mu_B \left(\left(\frac{S}{2B_0}\right)^2 - \frac{K}{B_0} \right) > 0 \tag{40}$$

which is possible with the appropriate choice of the parameters.

Section 6. Equations of motion in the linear approximation

The Lagrangian up to the second order in the unknowns is:

$$\begin{aligned} \mathcal{L}(x, y, z, \psi, \theta, \phi) &= \frac{1}{2} m (\dot{x}^2 + \dot{y}^2 + \dot{z}^2) \\ &+ \frac{1}{2} I_1 (\dot{\theta}^2 + \dot{\phi}^2) + \frac{1}{2} I_3 (\omega + \delta\dot{\psi} + \theta\dot{\phi})^2 - U(x, y, z, \delta\psi, \theta, \phi) \qquad (41) \end{aligned}$$

with

$$U = -mgz + \mu(B_x \theta + B_y \phi + B_z (1 - \frac{1}{2}\theta^2)(1 - \frac{1}{2}\phi^2) \tag{42}$$

Using the expressions for B_x, B_y, and B_z and retaining only the cuadratic terms:

$$U = -mgz + \mu(\frac{1}{2} S x \theta + \frac{1}{2} S y \phi + \frac{1}{2} B_0 (\theta^2 + \phi^2) \tag{43}$$

$$-Sz - Kz^2 + \frac{1}{2} K (x^2 + y^2)) \tag{44}$$

The Euler-Lagrange equations

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = 0 \tag{45}$$

with $q = (x,\ y,\ z,\ \psi,\ \theta,\ \phi)$, give:

$$m\ddot{x} = \frac{1}{2} \mu S \theta + \mu K x \tag{46a}$$

$$m\ddot{y} = \frac{1}{2} \mu S \phi + \mu K y \tag{46b}$$

$$m\ddot{z} = -2\mu K z \tag{46c}$$

$$I_1 \ddot{\theta} = I_3 \omega \dot{\phi} + \frac{1}{2} \mu S x + \mu B_0 \theta \tag{46d}$$

$$I_1 \ddot{\phi} = -I_3 \omega \dot{\theta} + \frac{1}{2} \mu S y + \mu B_0 \phi \tag{46e}$$

$$I_3 \delta\ddot{\psi} = 0 \tag{46f}$$

Section 7. Solutions in simple cases

1.- The vertical motion is governed by the equation

$$m\ddot{z} = -2\mu K z \tag{47}$$

which is the equation of a harmonic oscillator of frequency

$$\omega_z = \sqrt{2\mu K/m} \tag{48}$$

2.- Without magnetic field the non-trivial equations are:

$$I_1\ddot{\theta} = I_3\omega\dot{\phi} \tag{49}$$
$$I_1\ddot{\phi} = -I_3\omega\dot{\theta} \tag{50}$$

Introducing $v = \theta + i\phi$ we get

$$I_1\ddot{v} = -iI_3\omega\dot{v} \tag{51}$$

The solution of this equation is of the form $e^{i\alpha t}$. Substituting gives $\alpha = (I_3/I_1)\omega$. The functions θ and ϕ have the form:

$$\theta = A\cos(\alpha t + \delta) \tag{52}$$
$$\phi = A\sin(\alpha t + \delta) \tag{53}$$

In the linear approximation, the vector $\mathbf{n}$ is $\mathbf{n} = \theta\mathbf{e}_x + \phi\mathbf{e}_y + \mathbf{e}_z$. Therefore, this solution represents a precession of the top axis with angular velocity $(I_3/I_1)\omega$, which corresponds to a free top.

3.- For a constant field, following the same procedure as in point 2, we have:

$$I_1\ddot{v} = -iI_3\omega\dot{v} + \mu B_0 v \tag{54}$$

Neglecting the term on the left and assuming $v = v_0e^{i\alpha t}$ we obtain for α

$$\alpha = \frac{\mu B_0}{I_3\omega} \tag{55}$$

This is the precession velocity of the spinning top obtained in Section 5.

Section 8.Dispersion relation and lower limit of rotational speed

Introducing the variables $u = x + iy$ and $v = \theta + i\phi$, the equations of motion are:

$$m\ddot{u} = \frac{1}{2}\mu S v + \mu K u \tag{56}$$
$$I_1\ddot{v} = -iI_3\omega\dot{v} + \frac{1}{2}\mu S u + \mu B_0 v \tag{57}$$

We search for solutions of the form $u = u_0e^{i\alpha t}$ and $v = v_0e^{i\alpha t}$. The system of equations is transformed into a homogeneous system of algebraic equations for u_0 and v_0. For there to be a solution, the determinant of the coefficient matrix must be zero. This is:

$$\begin{vmatrix} \alpha^2 + \mu K/m & \frac{1}{2}\mu S/m \\ \frac{1}{2}\mu S/m & \alpha^2 + \alpha I_3\omega/I_1 + \mu B_0/I_1 \end{vmatrix} = 0 \tag{58}$$

The equation for α is:

$$(\alpha^2 + \mu K/m)(\alpha^2 + \alpha I_3\omega/I_1 + \mu B_0/I_1) = (\frac{1}{2}\mu S/m)^2 \tag{59}$$

For a uniform magnetic field:

$$\alpha^2 + \alpha I_3\omega/I_1 + \mu B_0/I_1 = 0 \tag{60}$$

whose solution is:

$$\alpha = \frac{1}{2}(-I_3\omega/I_1 \pm \sqrt{(I_3\omega/I_1)^2 - 4\mu B_0/I_1}) \tag{61}$$

For the roots to be real ω must satisfy:

$$\omega \geqslant 2\frac{\sqrt{\mu I_1 B_0}}{I_3} \tag{62}$$

For values smaller than this, there will be complex solutions of α with negative imaginary part, and small disturbances will grow exponentially, moving the top away from equilibrium.

Calculating the maximum speed for stability requires a more detailed analysis of the dispersion relationship.

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Physics at the nanoscale

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Nanomaterials in general, and nanoparticles and thin films in particular, are of extended use nowadays and among the most active research fields in materials sciences. In Physics, the interest in nanoscale systems lies in the new physical properties that emerge at small length scales. Moreover, these properties will be strongly dependent on size, surface-to-volume ratio, and shape. In the following exercises we will work on the physics behind the preparation of these nanomaterials and we will have a look at some of their special properties.

1. (1p.) Quantum dots (QDs) are solid crystalline particles with sizes in the order of the nanometer. When UV light hits these semiconducting nanoparticles, they can emit light of various colors. Some current applications for these nanoparticles are found in composites, solar cells and fluorescent biological labels. One of the methods for obtaining QDs is by controlled solidification from the liquid phase. When a liquid that is taken out of equilibrium (lowering the temperature, increasing pressure or increasing the amount of solute in case of more than one component), it will have an excess free energy per unit volume of Δg that will favour the phase transition. However, the apparition of clusters of the new phase, the solid crystal in this case, will involve the creation of an interface between the two phases, which has an energetic cost of σ (surface tension, units of energy per unit surface or Newton per metre). Imagine the situation in which the liquid is taken out of equilibrium and, by thermal fluctuations, an embryo of a crystal assembles in the liquid. **Considering the interplay between volume and surface energies and the embryo as spherical, which is the minimum radius that it must have so it is more energetically favourable for the system that the embryo continues growing instead of disappearing once it has already formed?** (Note: do not consider the change in configuration entropy in your calculations).

2. (1p.) Once the new particle has appeared it must grow up to a desired size, which will depend on the application. In multi-component systems usually the growth is diffusion controlled, since the new particle consumes part of the available solute at its nearby surroundings. Consider a **2D system** where a single circular nanoparticle of radius r' with constant concentration c_S (see figure 1) grows consuming part of the solute it has at its surroundings. At a certain distance $r' + \delta$ the concentration

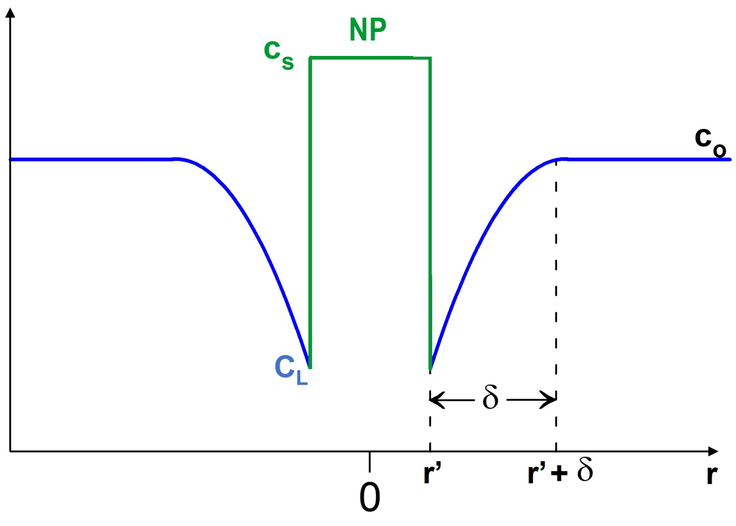

Figure 1: Concentration profile of a section of the nanoparticle and its surroundings. c_S denotes de concentration of the nanoparticle, c_L the concentration at the interface with the liquid and c_o the initial concentration of the liquid. The particle has radius r' and circular symmetry, so the concentration only depends on the distance from the center of the particle (no angular dependence).

recovers its overall concentration c_o. Just at the interface, the solid is in equilibrium with the liquid, so the liquid has a concentration c_L. **Considering this concentration profile as stationary ($\partial c/\partial t = 0$), use the two Fick's laws to calculate the growth rate, dr/dt.** Note: Consider the atoms that form the particle to have s_{at} as atomic surface (m^2/atom).

Fick's laws for diffusion: $\mathbf{J} = -D\nabla c$ and $\frac{\partial c}{\partial t} = D\Delta c$, where $\mathbf{J}$ is the atomic flux (in units of atoms/$(s \cdot m)$, since we are in 2D), D is the diffusion coefficient (m^2/s), c is the concentration (atoms/m^2 in 2D) and Δ is the Laplace operator.

3. (1p.) Due to curvature effects, the size of the nanoparticle has a strong influence on its melting point. In order to evaluate this effect, we can start by evaluating the difference in chemical potential when moving a differential of particles, dn from a flat surface ($r = \infty$) to the surface of a spherical particle of radius r. This difference in chemical potential for a spherical particle will increase the Gibbs free energy of the solid shifting the equilibrium temperature between the solid and the liquid. Remember that this temperature can be obtained from the Gibbs free energy from the difference in enthalpy and entropy between the liquid and the solid, $\Delta g = \Delta h - T\Delta s$, where Δg is the difference in Gibbs free energy per unit volume between the liquid and the solid and Δh and Δs are the difference in enthalpy and entropy per unit volume between the liquid and the solid. In particular, at the melting point of a bulk system, T_m, liquid and solid are in thermodynamic equilibrium and $\Delta g = \Delta h_m - T_m \Delta s_m = 0$, where Δh_m and Δs_m are, respectively, the melting enthalpy and entropy.

Evaluate the melting temperature shift of a spherical nanoparticle of radius r with respect to the bulk melting temperature ($r = \infty$). Consider that the system is not far away from the equilibrium point between liquid and solid, so the difference in enthalpy and entropy between the liquid and the solid can be assumed as constant, hence independent of temperature and equal to the melting enthalpy and entropy, Δh_m and Δs_m. **Express the result as a function of the melting entropy per unit volume, the surface tension and the radius of the particle.**

4. (1p.) In Nanotechnology, the most extended nanomaterials are thin films, where only one of the 3 dimensions is reduced to the nanoscale. Thin films have already been used for more than half a century in making electronic devices or optical coatings among other applications. When built thin enough, thin films behave as confined 2D systems. They are fabricated by the deposition of material atoms on a substrate. In this regard, molecular beam epitaxy (MBE) is a well established technique to obtain thin films with the appropriate morphological characteristics. In this technique, a material is evaporated and introduced into an ultra-high vacuum chamber. The flux of atoms/molecules arrives to a substrate, where they get adhered allowing the growth of the thin film following the crystal structure of the substrate. The flux of atoms that reach a surface (number of atoms/molecules hitting per unit time and surface) can be calculated from $F = \frac{1}{4} n v_a$ where v_a is the average speed of the gas molecules and n is the number of molecules per unit volume. Consider an ideal gas with a velocity that follows the Maxwell-Boltzmann distribution:

$$\rho(v) = 4\pi \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} v^2 \exp\left(-\frac{mv^2}{2kt}\right)$$

where m is the mass of one molecule, k is the Boltzmann constant and T stands for thermodynamic temperature. **Calculate the flux of molecules that arrive to the substrate as a function of pressure, temperature and mass of the molecules.**
Hint: $\int_0^\infty x^n \exp(-ax)\, dx = \frac{n!}{a^{n+1}} (n = 0, 1, 2, ...\mathrm{Re}(a) > 0)$

5. (1p.) When the gas molecules/atoms arrive to the substrate, some of them will lose part of their energy and will start forming a solid on the substrate surface (heterogeneous nucleation). As in exercise 1, the conditions must be energetically favorable for this phase transition (gas-solid) to take place. Moreover, instead of having just one type of surface σ_{sg} (substrate-gas), two new surfaces are emerging (σ_{cg} (crystal-gas) and σ_{sc} (substrate-crystal)), with their corresponding energetic cost. Let's consider that the new crystal has the shape of a spherical cap of height h, radius a, and radius of curvature r. The surface of the cap forms an angle θ with the surface, as shown in the figure. In the extreme of having a self-standing droplet, this angle would be π rad and we would recover the phase transformation studied in exercise 1 (homogeneous nucleation). Let's define ΔG as the difference in energy between a system that consists only of gas and substrate and one where one single droplet of radius of curvature r has formed on the surface. ΔG must take into account both the difference in free energy between the two phases and the energetic cost of all the different interfaces. **Prove that**

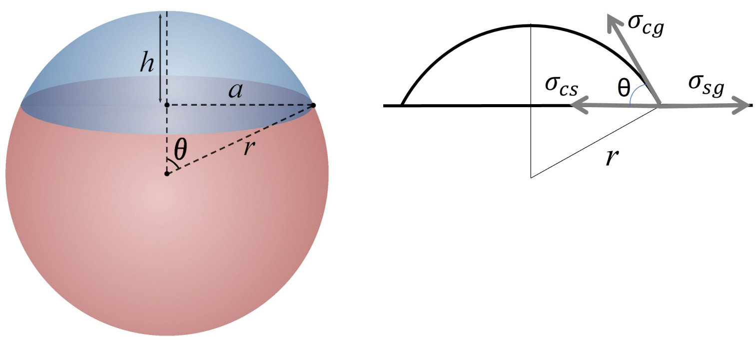

Figure 2: *Left*: Spherical cap of radius a, height h and radius of curvature r (Extracted from Wikipedia, author: Jhmadden. *Right*: Drawing of a solid droplet with the shape of a spherical cap. θ denotes the wetting angle. The arrows indicate the direction of the forces exerted by the different surface tensions.

ΔG_{het} (formation of the crystal on a surface) and ΔG_{hom} (self standing nucleus, $\theta = \pi$, as in exercise 1) are related following $\Delta G_{het} = f(\theta)\Delta G_{hom}$ where $f(\theta) = \frac{2-3\cos\theta+\cos^3\theta}{4}$. (Note: do not consider the effect of configuration entropy).
Hint: the volume and top surface of the cap from the figure can be calculated as $V = \frac{\pi}{3}r^3(2+\cos\theta)(1-\cos\theta)^2$ and $A = 2\pi r^2(1-\cos\theta)$

6. (1p.) Either if the film grows layer by layer or by the coalescence of the droplets, from a certain moment, a continuous film has formed. Films of several nanometers thick are of common use in the microelectronics industry. Therefore, let's consider we are working with a semiconductor material, where charge carriers have an effective mass m^* and can be considered as nearly free. For layers of a few nanometers, the film behaves as a 2D system from the perspective of charge carriers, which are quasi-free in the plane of the film (xy) and are confined in an infinite potential well of width a (the thickness per unit volume per unit energy of the film) in the z direction. **Calculate the density of states for electrons (number of electron states per unit volume per unit energy) as function of film thickness and of the effective mass of the electrons.**

7. (1p.) Without doping, a semiconductor is defined as intrinsic and has its Fermi energy right in the middle of the gap (typical values for a band gap in a semiconductor are around 1 eV). Still, at room temperature the conduction band will be populated with some electrons. **Calculate how many electrons per unit surface can be found in the conduction band as a function of the effective mass of electrons (m^*), the thickness of the film (a), the Fermi energy of the material (E_F) and the temperature (T) for the system described in exercise 6. You will need to make approximations to carry out the calculation, justify all of them.**(Hint: Boltzmann constant, $k = 8,617 \cdot 10^{-5} eV/K$)

8. (1p.) Doping semiconductors allows to have more charge carriers in the material. A way to introduce a different type of atom in the crystalline structure of the film is by depositing a film of the doping material on top of our semiconductor film. Since the diffusion coefficient, D, has an Arrhenius dependence with temperature, a subsequent increase of temperature would promote the diffusion of the doping atoms into the semiconductor layer. **Use Fick's laws to calculate the concentration profile in the semiconductor as function of time and depth.** For this calculation consider a **finite source** of doping atoms located at the surface, $c_o(x) = Q\delta(x)$ at $t = 0$ where Q denotes the released amount of atoms per unit cross-sectional area at $t = 0$. You can also consider the semiconductor film is infinitely thick to simplify the calculation and thus $\lim_{x\to\infty} c = 0$ for $t < \infty$. D can be considered constant since the experiment is carried on at constant temperature. Hint: You can try a function of the type $c(x,t) = t^a F(x^2/t^b)$ since $\lim_{t\to 0}\left[t^{-1/2}\exp\left(-x^2/t\right)\right] = \sqrt{\pi}\delta(x)$

9. (1p.) A way to further confine the carriers in our 2D semiconductor is applying a strong magnetic field, B, perpendicular to the plane of the sample. **You can use the Landau Gauge $\boldsymbol{A} = (0, Bx, 0)$ as the vector potential for a magnetic field applied in the z direction to**

calculate the energy of the fundamental state considering that electrons are confined in the z direction in an infinite potential square well. Express the result as function of m^*, a (the thickness of the film), and B. (Obviously, other constants such as the Planck's constant or the charge of the electron can be present in the result).

10. (1p.) Let's give some numbers to the previous exercise. The application of the magnetic field gives raise to a quantification of the energy of the carriers, in what are called Landau energy levels. **If we go to a temperature close to 0 K and apply a magnetic field of 10 T perpendicular to our film, the carrier with the highest energy will have an energy of $12E_o$, where $E_o = \frac{\pi^2\hbar^2}{2m^*a^2}$, with $a = 10$ nm. How many Landau levels will be filled under these conditions? Consider spin degeneration.** ($\hbar = 1,054 \cdot 10^{-34} J \cdot s$, $m^* = 0.067 m_o$, $m_o = 9,1 \cdot 10^{-31} kg$).

Solution

1. (1p.) We have to calculate in first place the difference in energy between the liquid, which has been taken out of equilibrium, and the liquid in which a cluster has formed by a statistical fluctuation. This difference in energy can written as:

$$\Delta G = \frac{4}{3}\pi r^3 \Delta g + 4\pi r^2 \sigma$$

The cluster is in equilibrium, so Δg is negative. Since σ is always positive, ΔG will present a maximum for a certain value of r. For smaller r, the growth of the cluster would mean an increase of ΔG, so the cluster will shrink until disappearing. On the other hand, for clusters with larger r, it will be energetically favourable for the cluster to grow. This critical r can be found from the derivative of ΔG:

$$r_c = -\frac{2\sigma}{\Delta g}$$

2. (1p.) Since we are in 2D and the particle is circular, it is convenient to work in polar coordinates. We can rewrite Fick's laws in the following way:

$$J_{matter} = 2\pi r D \frac{\partial c}{\partial r}$$

$$\frac{\partial c}{\partial t} = D \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial c}{\partial r} \right)$$

where the derivatives in the polar angle are zero due to circular symmetry and the flux is calculated as the amount of matter (atoms) that crosses the interface of a circular particle of radius r. Thus, the initial flux from Fick's law has been multiplied by the length of the circumference ($2\pi r$) and the minus sign has been removed to have the number of atoms per unit time that arrive to the nanoparticle.

Considering stationary state, circular symmetry and that r must be different from zero, $r\frac{\partial c}{\partial r} = B$ must be constant. This constant can be found by integrating and imposing the boundary conditions from the exercise: $c = c_L$ for r equal to the actual radius of the particle and $c = c_o$ for $r = r + \delta$. In this way, we find $B = \frac{c_o - c_L}{\ln\left(\frac{r+\delta}{r}\right)}$. The flux of matter is, therefore:

$$J_{matter} = 2\pi D \frac{c_o - c_L}{\ln\left(\frac{r+\delta}{r}\right)}$$

To calculate the growth rate we can make an estimation of the number of atoms in the particle by $N = \frac{\pi r^2}{s_{at}}$. Considering that matter is preserved, the amount of atoms that will arrive to the particle J_{matter} must be equal to the variation of N as a function of time, $J_{matter} = \frac{dN}{dt}$. From the derivative of N we get dr/dt and finally:

$$\frac{dr}{dt} = \frac{D s_{at}(c_o - c_L)}{r \ln\left(\frac{r+\delta}{r}\right)}$$

3.(1p.) The difference in chemical potential between a spherical particle of radius r and the bulk can be estimated from the difference in free energy when moving a differential of atoms, dn, from a flat to a spherical surface with radius of curvature r:

$$\Delta \mu = \mu_r - \mu_\infty = \sigma \frac{dA}{dn}$$

where μ_r and μ_∞ are the chemical potential of the equilibrium phase (the crystal) for a spherical drop of radius r and for a crystal with no curvature, respectively. Since both systems are in equilibrium, the only difference comes from building extra surface, dA, in the case of the spherical droplet with an associated surface tension σ. dn will increase the volume of the droplet by $dV = dn/\Omega$, where Ω is the atomic volume. We can assume that this volume will get distributed homogeneously along all the surface, so $dV = 4\pi r^2 dr$. On the other hand, the variation of the area when increasing the radius a dr can be written as $dA/dr = 8\pi r$. Using these relations we find that $dA/dn = 2\Omega/r$ for a spherical particle. Therefore, the difference in chemical potential can be written as $\Delta\mu = 2\sigma\Omega/r$.

A spherical particle will have this extra energy term that depends on the size of the particle through the radius of curvature. This extra energy shifts the equilibrium free energy of the solid, and therefore, the crossover between the equilibrium lines of solid and liquid (in the Gibbs free energy phase diagram) will occur at a different temperature, shifting the melting temperature of the system. In a single component system, the chemical potential and the Gibbs free energy per unit volume,Δg, can be related by $\Delta\mu = \Omega\Delta g$. Then, from the previous calculation we get $\Delta g = 2\sigma/r$. We can calculate the new melting temperature, T_r from $\Delta g = \Delta h - T_r\Delta s$, where Δh and Δs are respectively the enthalpy and entropy difference between the liquid and the solid per unit volume at T_r. In this way, we can finally write

$$\frac{2\sigma}{r} = \Delta h - T_r \Delta s \tag{1}$$

which will give us the new melting temperature, T_r for a particle of radius r.

According to the exercise, we are not far from equilibrium, so we can consider that both enthalpy and entropy differences do not differ considerably from the ones at the equilibrium melting temperature, T_m, i.e. when the radius of curvature is infinite (flat surface). So $\Delta h = \Delta h_m$, $\Delta s = \Delta s_m$ and $\Delta g = \Delta h_m - T_m\Delta s_m = 0$ defines the melting temperature of a system with an infinite radius of curvature. Isolating $Deltah_m$ from the last expression, we get $\Delta h_m = T_m\Delta s_m$. Using this expression in equation 1 and rearranging the different terms, we finally get:

$$T_m - T_r = \frac{2\sigma}{r\Delta s_m}$$

4.(1p.) To calculate the flux, we first need the average speed of the gas molecules, v_a, which can be obtained from the velocity distribution $\rho(v)$:

$$v_a = \int_0^\infty v\rho(v)\,dv = \int_0^\infty 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2} v^3 \exp\left(-\frac{mv^2}{2kT}\right) dv$$

To simplify the integral we can write $a = 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2}$ and $b = m/2KT$. In this way:

$$v_a = a\int_0^\infty v^3 e^{-bv^2}\,dv$$

We can apply the following substitution: $u = v^2$, $du = 2vdv$

$$v_a = \frac{a}{2}\int_0^\infty ue^{-bu}\,du$$

Integrating, we get $v = \frac{a}{2b^2}$, so $v_a = \sqrt{\frac{8kT}{\pi m}}$

Once we have v_a, we need to obtain an expression for n. We can use the ideal gas law, written as $P = nkT$, where n is the number of atoms per unit volume. According to the exercise, the flux could be written as $F = \frac{1}{4}nv_a$, so we can finally write

$$F = \sqrt{\frac{P^2}{8KT\pi m}}$$

5. We have to demonstrate that $\Delta G_{het} = f(\theta)\Delta G_{hom}$ for a spherical cap with a radius of curvature r and a wetting angle θ as indicated in the figure. We calculate ΔG_{het} in the first place. Taking into account the geometry of the problem and the considerations of exercise 1:

$$\Delta G_{het} = V_{cap}\Delta g + A_{cap}\sigma_{cg} + A_s(\sigma_{cs} - \sigma_{sg})$$

where V_{cap} is the volume of the spherical cap, A_{cap} is the surface of the cap, which corresponds to the interface crystal-gas, and A_s is the contact surface of the cap with the substrate. These volumes and areas can be written as a function of the radius of curvature and the wetting angle as:

$$V_{cap} = \frac{\pi r^3}{3}(2 - 3\cos\theta + \cos^3\theta)$$

$$A_{cap} = 2\pi r^2(1 - \cos\theta)$$
$$A_s = \pi a^2 = \pi r^2(1 - \cos^2\theta)$$

From the surface tension drawing, if the system is in dynamic equilibrium, one can also see that $\sigma_{cs} + \sigma_{cg}\cos\theta = \sigma_{sg}$, so $\sigma_{cs} - \sigma_{sg} = -\sigma_{cg}\cos\theta$.

We can rewrite now the ΔG_{het} as

$$\Delta G_{het} = \frac{\pi r^3}{3}(2 - 3\cos\theta + \cos^3\theta)\Delta g + \sigma_{cg}(-\pi r^2\cos\theta(1 - \cos^2\theta) + 2\pi r^2(1 - \cos\theta))$$

By rearranging the different terms, one can obtain:

$$\Delta G_{het} = \frac{1}{4}(2 - 3\cos\theta + \cos^3\theta)\left[\frac{4\pi r^3}{3}\Delta g + 4\pi r^2\sigma_{cg}\right]$$

which is precisely $\Delta G_{het} = f(\theta)\Delta G_{hom}$

6.(1p.) The density of states, $g(E)$ can be obtained from the number of states per unit volume (or surface, in 2D) up to a certain energy E, $n(E)$, as $g(E) = \frac{\partial n(E)}{\partial E}$. To calculate the number of states one can start working in the reciprocal space. Since we are in 2D and in the quasi-free electron model, we can work in polar coordinates and calculate the number of states contained in a circle of radius k, where k is the momentum.

$$N(k) = 2\frac{\pi k^2}{\frac{(2\pi)^2}{S}}$$

where 2 accounts for the spin, and $\frac{(2\pi)^2}{S}$ is the area occupied by each k state. Therefore, the number of k states per unit surface will be $n(k) = \frac{k^2}{2\pi}$. Introducing here the energy dispersion relation for quasi-free electrons, $E = \frac{\hbar^2 k^2}{2m*}$, one obtains $n(E) = \frac{m^* E}{\pi\hbar^2}$. By deriving the number of states we get the density of states for a 2D system $g(E) = \frac{m^*}{\pi\hbar^2}$.

However, the carriers only behave as free in the xy plane. In the z direction the carriers are confined in an infinite square well potential. In this direction, we will have discrete energy levels. Thus, the density of states we have just calculated is the one associated to each of the energy levels in the z direction. Therefore, the final energy of states is

$$g(E) = \frac{m^*}{\pi\hbar^2}\sum_{n=1}^{\infty}\Theta(E - E_n)$$

where $\Theta(E - E_n)$ is the Heaviside step function and E_n are the discrete energy levels of the infinite square well, $E_n = \frac{n^2\pi^2\hbar^2}{2m^*a^2}$.

7.(1p.) Without doping, the Fermi energy, E_F, is located at the middle of the gap. Thermal energy, kT, will provide enough energy for some of the carriers to transit into the conduction band. The total number of carriers per unit surface in the conduction band can be calculated by

$$n = \int_{E_c}^{\infty} g(E) f_{FD}(E, E_F)\, dE$$

where E_c is the bottom of the conduction band, $f_{FD}(E, E_F)$ is the Fermi-Dirac distribution function and $g(E)$ is the density of states. Considering that at room temperature $kT \sim 25meV$ is much smaller than the distance between the Fermi energy and the bottom of the conduction band, the Fermi-Dirac distribution function for energies above E_c can be approximated to the Maxwell-Boltzmann distribution function

$$f_{FD}(E, E_F) = \frac{1}{e^{\frac{E-E_F}{kT}} + 1} \approx e^{-\frac{E-E_F}{kT}} \quad \text{if} \quad \frac{E-E_F}{kT} >> 1$$

Thus, the number of states above E_c can be written as

$$n = \int_{E_c}^{\infty} g(E) \exp\left(-\frac{E-E_F}{kT}\right) dE$$

Since we have discrete energy levels in the z direction, the carriers won't be allowed to have energies starting from E_c but from E_1, the first energy level of the infinite square well. Moreover, we have to calculate the amount of carriers for each of these discrete levels. So, for level i,

$$n_i = \int_{E_i}^{\infty} g(E) \exp\left(-\frac{E-E_F}{kT}\right) dE$$

with $g(E) = \frac{m^*}{\pi\hbar^2}$.

This integral yields

$$n_i = \frac{m^* kT}{\pi\hbar^2} e^{-\frac{E_i - E_F}{kT}}$$

The total number of carriers in the conduction band will be, therefore

$$n = \sum_{i=1}^{\infty} \frac{m^* kT}{\pi\hbar^2} e^{-\frac{E_i - E_F}{kT}}$$

with $E_i = \frac{i^2\pi^2\hbar^2}{2m^* a^2}$.

8.(1p.) This is a 1D problem, since the net flux will be towards the inside of the film. Therefore, to solve this problem we will use Fick's second law in one dimension:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

where $x = 0$ will be located at the surface of the film and x will increase with depth. For simplicity, it is better to solve the differential equation considering an infinite domain, that goes from $-\infty$ to ∞. So we will consider an initial load of atoms of $2Q$ instead of Q that will diffuse towards $+x$ and $-x$.

The boundary conditions are as follows:

$$c = c_o(x) = 2Q\delta(x) \quad \text{at} \quad t = 0$$

$$\lim_{x\to\infty} c = \lim_{x\to-\infty} c = 0 \quad \text{for} \quad t < \infty$$

where Q is the released amount of atoms per unit cross-sectional area and $\delta(x)$ is the Dirac delta function.

The solution must be symmetric in the $+x$ and $-x$ directions and must have a peak shape with constant area (equal to the total amount of released atoms) but with a maximum that decreases with time. Using the function suggested in the exercise:

$$c(x,t) = t^{-\alpha} F(\phi) \quad \text{with} \quad \phi = \frac{x^2}{BDt}$$

where $\alpha > 0$ is the size factor and $F(\phi)$ is the shape factor, which will provide a similar peak profile $\forall t$. In ϕ, B is a constant and D is the diffusion coefficient, which makes ϕ dimensionless and contributes by spreading the peak faster if D is higher. The fact of having x^2 and t is an educated guess, based on the second and first derivatives for x and t, respectively.

In this way, we can calculate the partial derivatives:

$$\frac{\partial c}{\partial t} = -\alpha t^{-\alpha-1}F(\phi) - t^{-\alpha-1}\phi\frac{dF(\phi)}{d\phi}$$

$$\frac{\partial^2 c}{\partial x^2} = \frac{2t^{-\alpha-1}}{BD}\frac{dF}{d\phi} + t^{-\alpha-1}\frac{4}{BD}\phi\frac{d^2F}{d\phi^2}$$

Applying them to Fick's second law we finally get:

$$\phi\frac{d}{d\phi}\left(F + \frac{dF}{d\phi}\right) + \frac{1}{2}\left(\frac{dF}{d\phi} + 2\alpha F\right) = 0$$

where we can take the constant $B = 4$ for convenience. Since α is still free, we can take it as $1/2$ and the solution will be of the type:

$$F + \frac{dF}{d\phi} = 0$$

which has the solution $F(\phi) = A\exp(-\phi)$.

Therefore, the concentration can be written as

$$c(x,t) = At^{-1/2}\exp\left(-\frac{x^2}{4Dt}\right)$$

To calculate A, we must go back to the original boundary conditions and impose that the total amount of atoms must be equal to 2Q:

$$\int_{-\infty}^{\infty} c(x,t)\,dx = \int_{-\infty}^{\infty} c_o\,dx = \int_{-\infty}^{\infty} 2Q\delta(x)\,dx = 2Q$$

With this condition we get $A = \frac{2Q}{\sqrt{4\pi D}}$.

Going back to a problem that goes from $x = 0$ to ∞, the final solution is:

$$c(x,t) = \frac{Q}{\sqrt{4\pi Dt}}\exp\left(\frac{-x^2}{4Dt}\right)$$

9.(1p.) To find the energy after confining with a magnetic field we need to introduce the magnetic field as a potential in Schrödinger's equation. We can do that by using the Landau Gauge:

$$\overrightarrow{A} = (0, Bx, 0) \quad \text{where} \quad \overrightarrow{B} = \nabla \times \overrightarrow{A}$$

We can now introduce in Schrödinger's equation this vector potential and the confinement potential in the z direction:

$$\left[\frac{1}{2m^*}(\hat{p} - q\overrightarrow{A})^2 + V(z)\right]\Psi(x,y,z) = E_{xyz}\Psi(x,y,z)$$

where $\hat{p} = -i\hbar\nabla$ is the canonical momentum. By using the Landau Gauge, we get

$$\left[\frac{-\hbar^2}{2m^*}\nabla^2 - \frac{ie\hbar Bx}{m^*}\frac{\partial}{\partial y} + \frac{(eBx)^2}{2m^*} + V(z)\right]\Psi(x,y,z) = E_{xyz}\Psi(x,y,z)$$

since movement in the z direction is not affected by the field, we can consider

$$\Psi(x,y,z) = \psi(x,y)u(z) \quad \text{and, therefore,} \quad E_{xyz} = E_{xy} + E_z$$

In the z direction we have the solutions for $u(z)$ and E_z of the infinite square well. In the xy plane, we have

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}-\frac{ie\hbar Bx}{m^*}\frac{\partial}{\partial y}+\frac{(eBx)^2}{2m^*}\right]\psi(x,y)=E_{xy}\psi(x,y)$$

Since the vector potential does not depend on y, the solution is of the type $\psi(x,y)=\phi(x)e^{iky}$ and Schrödinger's equation can be written as a function of x only:

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m^*\omega_c^2\left(x+\frac{\hbar k}{eB}\right)^2\right]\phi(x)=E_{xy}\phi(x)$$

with $\omega_c=\frac{eB}{m^*}$. This is the equation of a harmonic oscillator, where $\phi(x)$ are the Hermite polynomials and the energy takes discrete values, corresponding to the Landau energy levels

$$E_{xy}=\hbar\omega_c\left(n-\frac{1}{2}\right)\quad\text{with}\quad n=1,2,3...$$

This is the energy associated to the xy dimension, so we still have to add the one corresponding to the confinement in the z direction. Since in the z direction we have an infinite square well, the energy can written as

$$E=E_{xy}+E_z=\hbar\omega_c\left(n-\frac{1}{2}\right)+\frac{i^2\pi^2\hbar^2}{2m^*a^2}\quad\text{with}\quad n=1,2,3...\quad\text{and}\quad i=1,2,3...$$

The lowest energy state possible would have $n=i=1$.

10.(1p.) First of all we need to analyze how the different discrete energy levels will be filled. We will start filling the first energy level of the infinite square quantum well, which has an energy of E_o according to the exercise. Then, we start filling the different Landau energy levels. For each $\hbar\omega_c$ in energy, we will fill another level. Therefore, for the first level of the infinite well, $i=1$, we will be able to fill

$$n_{LL}(i=1)=\frac{12E_o-E_o}{\hbar\omega_c}$$

Following the same reasoning, for the next levels of the square well we have:

$$n_{LL}(i=2)=\frac{12E_o-4E_o}{\hbar\omega_c}$$

$$n_{LL}(i=3)=\frac{12E_o-9E_o}{\hbar\omega_c}$$

The next level, $i=4$, can not be filled, since the energy of the level is lower than the one of the electron with the highest energy. In this calculation we are considering that each Landau level holds both spin up and spin down. Substituting the values provided by the exercise:

$$n_{LL}(i=1)=35,71\quad n_{LL}(i=2)=25,97\quad n_{LL}(i=3)=9,74$$

Estudiantes R.S.E.F.

Preliminares PLANCKS 2023

The gravity of neutron waves

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The perfect-silicon-crystal interferometer was first developed for x rays by Bonse and Hart in 1965 (1). Ten years later, Colella, Overhauser and Werner (2) used this device to make the first observation of the gravitationally-induced quantum interference of neutron waves (questions d. and e.). The inertial effect on the neutron phase due to the rotation of the Earth has also been detected by Werner, Staudenmann and Colella (questions g. and h.) A delightful account of how the COW experiment happened can be found in (4). A very readable description of these early stages of neutron interferometry can be found in (5).

(1) U. Bonse and M. Hart, Appl. Phys. Lett. 69 155 (1965).
(2) R. Colella, A.W. Overhauser and S.A. Werner, Phys. Rev. Lett. 34 (1975) (3) S.A. Werner, J.-L. Staudenmann and R. Colella, Phys. Rev. Lett. 42 (1979) 1103.
(4) R. Colella and A.W. Overhauser, Physica B 385–386 (2006) 1408–1410. Available online at www.sciencedirect.com
(5) S. A. Werner, Physics Today 33, 12, 24 (1980).

In this problem we will consider thermal neutrons with wavelengths of the order of the spacing of crystalline lattices (a fewÅ), propagating inside devices with sizes of the order of a few cm. These wavelengths and sizes, are known in the experiment with three significant figures. For simplicity, unless otherwise stated we will consider all waves here as monochromatic plane waves.

A horizontal beam of neutrons with wavelength λ is prepared. To see if the error incurred by treating its path as a straightline path of free particles is acceptable;

a. (0.5 points) Determine $(\delta z/x)$ and $\delta\theta$, where δz is the vertical deflection and $\delta\theta$ the angle that the beam direction forms with the horizontal after having traveled a horizontal distance x. Determine the errors $(\delta p/p)$ and $(\delta\lambda/\lambda)$ induced in the momentum and wavelength of the neutrons under these conditions.

Give the answers in terms of the wavelength, λ[Å] in Amstrongs, the distance, x[cm] in cm, and the numerical coefficients resulting from your calculation. The relevant parameters are given in the table with four significant digits.

Planck constant	h	6.626×10^{-34}	J Hz^{-1}
	$\hbar$	1.054×10^{-34}	J s
acceleration of gravity	g	9.806	m s^{-2}
neutron mass	m	1.674×10^{-27}	kg
neutron velocity	$v = h/(m\lambda)$	$3956/\lambda$[Å]	m s^{-1}

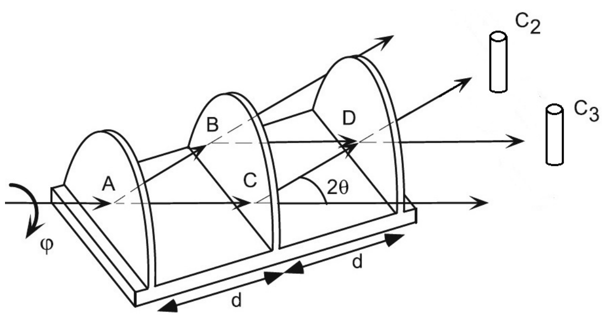
The small deviations from the horizontal have a counterpoint in the wave functions; the Schrödinger equation is

$$(H_0 + V)\psi = E\psi, \quad \text{with } H_0\psi_0 = E\psi_0,\ \psi_0 = e^{i\mathbf{k}_0\cdot\mathbf{r}},$$

$H_0 = (-\hbar^2/2m)\nabla^2$ is the free Hamiltonian and $V = mgz$ the gravitational potential.

b.1 (0.7 points) Obtain an approximate solution to the complete problem of the form $\psi = \psi_0\chi, E = E_0$, with $\psi_0 = e^{i\mathbf{k}_0\cdot\mathbf{r}}$, and χ such that $-\nabla^2\chi \ll k_0^2\chi$ can be neglected. Take $\mathbf{k}_0 = k\hat{\mathbf{e}}_x$ horizontal.

b.2 (0.3 points) Calculate the momentum $\hbar\mathbf{k}$ obtained from ψ and compare it with the classical value.



Sketch of the interferometer used in the COW experiment with two wide grooves between three plates. The incident beam directed along $\overline{AC}$ was kept horizontal throughout the experiment.

The first observation of the phase shift of a de Broglie neutron wave induced by Earth's gravity was made in an experiment conducted at the University of Michigan in 1975 by Colella, Overhauser, and Werner. In the experiment, a collimated monochromatic beam of neutrons of wavelength $\lambda = 1.445$Å is incident under Bragg conditions in a perfect silicon monocristal with two wide grooves carved like the one shown in the figure. During the experiment the whole setup was rotated around $\overline{AC}$ that was kept horizontal.

The incident beam at A is split by 'Bragg reflection' in the first Si crystal plate[1] producing transmitted and reflected beams in the incident and refected directions which are coherent. These are subsequently Bragg reflected in the middle crystal plate at points B and C. Two of the resulting beams

[1] The experiment uses Bragg reflection in the (220) lattice planes of the Si crystal. The Bragg angle is $\theta = 22.1°$, the distance between plates $d = 3.5$ cm. Henceforth we neglect the thickness of the plates.

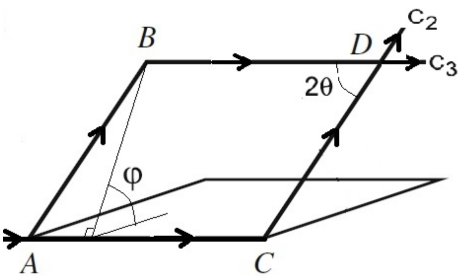
are directed towards point D in the third crystal plate, where they mix and interfere. The outgoing beams entering the two He gas-filled proportional detectors C_2 and C_3 are linear combinations of the waves traversing paths ABD and ACD.

The transmitted and reflected waves in each plate get complex transmission and reflection amplitudes, $a_t = t\, a_{in}$, $a_r = r\, a_{in}$, with $t = \cos\phi$ and $r = i\sin\phi$, where the angle ϕ is real. Take the incoming wave at A to be $\psi_0 = a_{in}e^{i\mathbf{k}_0\cdot\mathbf{r}}$ with $a_{in} = 1$ in arbitrary units, and set the origin of coordinates at point A. Label the paths ACD and ABD with the subscripts I and II respectively. Call L the side of the parallelogram $ABCD$. The parallelogram will be kept horizontal, $\varphi = 0$, in questions **c.n**) below.

c.1 (0.25 points) Write the waves at the input of the final plate, $\psi_{\text{I in}D}\,\psi_{\text{II in}D}$.

c.2 (0.25 points) Write out the waves ψ_2, ψ_3 **leaving the final plate towards the detectors** C_2 **and** C_3.

c.3 (0.5 points) Give the intensities I_2 **and** I_3 **measured in the detectors in terms of the transmission and reflection coefficients** T **and** R.



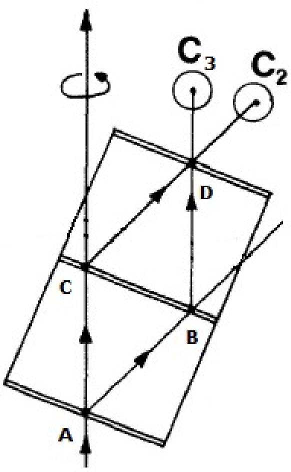
Tilted configuration by rotating the setup by an angle φ around the horizontal input direction $\overline{AC}$

The basic idea of the COW experiment is to tilt the interferometer about the incident beam line $\overline{AC}$ while maintaining the Bragg condition, causing a gravitationally-induced phase shift of the neutron deBroglie waves. So, the full parallelogram is in a tilted plane and the path $\overline{BD}$ is at a different height than $\overline{AC}$. Consider the case where the interferometer is rotated by an angle φ around $\overline{AC}$.

d. (1 point) Repeat c.1,2, showing the emergence at D **of a phase shift** δ **when the interferometer is tilted about the horizontal beam line** $\overline{AC}$ **by an angle** φ**. Calculate** δ. (Avoid calculating unnecesary integrals)

e. (1 point) Give I_2 **and** I_3 **in terms of** T **and** R**. Determine the number of fringes that will occur during a** $180°$ **rotation of the interferometer.**

During the experiment the interferometer was at rest in the laboratory frame and therefore rotating with the angular velocity of the Earth $\boldsymbol{\Omega}$.



Setup for question **h.** The interferometer rotates around the vertical direction $\overline{AC}$.

f. (0.5 points) Write the momentum of the neutrons including the term due to the rotation of the reference frame of the interferometer.

g. (1 point) Show that δ_Ω **can be written for any given orientation of the parallelogram using a surface integral S, yielding**

$$\delta_\Omega = \frac{2m}{\hbar}\boldsymbol{\Omega}\cdot\mathbf{S}.$$

Indicate the direction of the vector S and give its value in terms of d **and** θ.

In an experiment, carried out in Columbia (Missouri, USA) at latitude $\Phi = 38.63°$ with an interferometer of area $S = 8.864$ cm^2 the incident beam was kept vertical.

h. (1 point) Determine the number of fringes registered in the detectors when the interferometer was initially set in the local meridian plane and was rotated $12°$ **about the vertical direction** $\overline{AC}$ **from there.**

Finally, you are asked to analyze how it is possible for waves incident on a crystal at a certain angle θ_B to emerge on the other side partly transmitted and partly reflected forming precisely an angle $2\theta_B$. The asymptotic form of the wave function at large distance r from the scattering center can be written in the Born approximation as [2]

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} + f(\Delta\mathbf{k})\frac{e^{ikr}}{r}, \text{ with } f(\Delta\mathbf{k}) = -\frac{m}{2\pi\hbar^2}\int d^3r' V(\mathbf{r}')e^{-i\Delta\mathbf{k}\cdot\mathbf{r}'},$$

where $|\mathbf{k}| = |\mathbf{k}_0| = k$. The goal here is to check if the scattering amplitude $f(\Delta\mathbf{k})$ is only appreciable for momentum transfers $\Delta\mathbf{k} = \mathbf{k} - \mathbf{k}_0$, that fulfill the Bragg condition.

The atoms of the periodic crystal are located at $\mathbf{r}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_2\mathbf{a}_2$ with the n_i integers. The potential is periodic $V(\mathbf{r}_n + \mathbf{r}) = V(\mathbf{r})$.

i. (1 point) Show that the scattering amplitude can be factored into an integral over the unit cell and a sum of phase factors. Use the notation $\mathbf{r} = \mathbf{r}_n + \mathbf{x}$ where $\mathbf{x}$ is a position within the unit lattice.

j. (1 point) Use the Poisson summation formula

$$\sum_{n=-\infty}^{+\infty} e^{ixan} = \frac{2\pi}{|a|}\sum_{m=-\infty}^{+\infty}\delta(x - \frac{2\pi}{a}m)$$

to show that in the limit of infinite number of scatterers $n_i \in (-\infty, +\infty)$ the scattering amplitude would be strictly zero for momentum transfers $\Delta\mathbf{k}$ that do not belong to the reciprocal lattice,

k. (1 point) Use the above result to obtain the Bragg reflection formula.

[2] This approximation underestimates the dynamics of the neutrons within the crystal as well as the finite size of the crystal.

Solution

In this problem we will consider thermal neutrons with wavelengths of the order of the spacing of crystalline lattices (a fewÅ), propagating inside devices with sizes of the order of a few cm. These wavelengths and sizes, are known in the experiment with three significant figures. For simplicity, unless otherwise stated we will consider all waves here as monochromatic plane waves.

A horizontal beam of neutrons with wavelength λ is prepared. To check if the error incurred by treating its path as a straightline path of free particles is acceptable;

a. (0.5 points) Determine $(\delta z/x)$ and $\delta\theta$, where δz is the vertical deflection and $\delta\theta$ the angle that the beam direction forms with the horizontal after having traveled a horizontal distance x. Determine the errors $(\delta p/p)$ and $(\delta\lambda/\lambda)$ induced in the momentum and wavelength of the neutrons under these conditions.

Give the answers in terms of the wavelength, λ[Å] in Amstrongs, the distance, x[cm] in cm, and the numerical coefficients resulting from your calculation. The relevant parameters are given in the table with four significant digits.

Parabolic motion kinematics gives $x = vt$, $z = -\frac{1}{2}gt^2 \Rightarrow \delta z = \frac{1}{2}g\left(\frac{x}{v}\right)^2$. Using that $v = h/(m\lambda)$,

$$\frac{\delta z}{x} = \frac{g\ x}{2v^2} = \frac{m^2\lambda^2 g}{2h^2}\ x = 0.3133 \times 10^{-8}\ \lambda[\text{Å}]^2\ \ x[\text{cm}];\ \ \delta\theta \approx v_z/v_x = 2\delta z/x = 0.6266\ \times\ 10^{-8} rad$$

From energy conservation, $p'^2 - p^2 = 2m^2 g(z - z') \Rightarrow \delta p \approx \frac{m^2 g}{p}\delta z$. Thus,

$$\frac{\delta p}{p} = \frac{\delta\lambda}{\lambda} = \frac{g}{v^2}\left(\frac{\delta z}{x}\right)\ x = 0.1963 \times 10^{-16}\lambda[\text{Å}]^4\ x[\text{cm}]^2$$

These values indicate that the approximation of straight trajectories and constant λ or p can be used.

Planck constant	h	6.626×10^{-34}	J Hz^{-1}
	$\hbar$	1.054×10^{-34}	J s
acceleration of gravity	g	9.806	m s^{-2}
neutron mass	m	1.674×10^{-27}	kg
neutron velocity	$v = h/(m\lambda)$	$3956/\lambda$[Å]	m s^{-1}

The small deviations from the horizontal have a counterpoint in the wave functions; the Schrödinger equation is

$$(H_0 + V)\psi = E\psi, \quad \text{with}\ \ H_0\psi_0 = E\psi_0,\ \psi_0 = e^{i\mathbf{k}_0\cdot\mathbf{r}},$$

$H_0 = (-\hbar^2/2m)\nabla^2$ is the free Hamiltonian and $V = mgz$ the gravitational potential.

b.1 (0.7 points) Obtain an approximate solution to the complete problem of the form $\psi = \psi_0\chi, E = E_0$, with $\psi_0 = e^{i\mathbf{k}_0\cdot\mathbf{r}}$, and χ such that $-\nabla^2\chi \ll k_0^2\chi$ can be neglected. Take $\mathbf{k}_0 = k\hat{\mathbf{e}}_x$ horizontal.

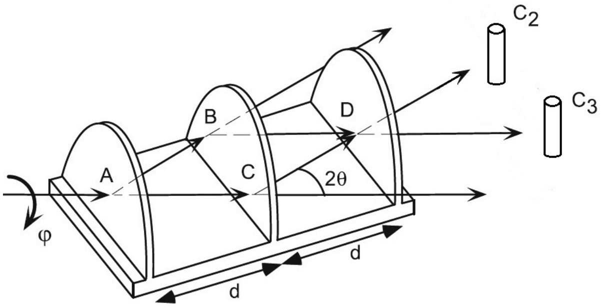
$$(H_0 + V)\psi_0\chi = E\psi_0\chi \Rightarrow i\frac{\hbar^2}{m}\mathbf{k}_0\cdot\nabla\chi + i\frac{\hbar^2}{2m}\nabla^2\chi = V\chi \longrightarrow \mathbf{k}_0\cdot\nabla\chi = -i\frac{m}{\hbar^2}V\chi.$$

With $\mathbf{k}_0 = k\hat{\mathbf{e}}_x$, $\chi = e^{-i\frac{m}{\hbar^2 k}\int_0^x dx V}$. Note that due to the scalar product, the integral is along the x axis. Substituting $V = mgz$ gives $\chi = e^{-i\frac{m^2 g}{\hbar^2 k}xz}$. Then,

$$\psi = e^{i(kx - \frac{m^2 g}{\hbar^2 k}xz)}$$

b.2 (0.3 points) Calculate the momentum $\hbar$k obtained from ψ and compare it with the classical value. According to question a. $\mathbf{p}_{classic}(x) = p\ \hat{\mathbf{e}}_x - \frac{m^2 g}{p}x\ \hat{\mathbf{e}}_z$; question b.1 gives

$$\mathbf{p}(x) = -i\hbar(\nabla\psi)/\psi = (p - \frac{m^4 g^2}{2p^3}x^2)\ \hat{\mathbf{e}}_x + \frac{m^2 g}{p}x\ \hat{\mathbf{e}}_z = \mathbf{p}_{classic}(x) + \mathcal{O}(g^2)$$



Sketch of the interferometer used in the COW experiment with two wide grooves between three plates. The incident beam directed along $\overline{AC}$ was kept horizontal throughout the experiment.

The first observation of the phase shift of a de Broglie neutron wave induced by Earth's gravity was made in an experiment conducted at the University of Michigan in 1975 by Colella, Overhauser, and Werner. In the experiment, a collimated monochromatic beam of neutrons of wavelength $\lambda = 1.445$Å is incident under Bragg conditions in a perfect silicon monocristal with two wide grooves carved like the one shown in Figure 2. During the experiment the whole setup was rotated around $\overline{AC}$ that was kept horizontal.

The instrument is made from a large and highly perfect single-crystal block. By cutting two wide grooves in the block, different parts of the same crystal can consecutively serve as a beam splitter, as two transmission mirrors, and as an analyzer crystal. In this way the very important spatial lattice coherence between all three plates can easily be maintained over long periods of time.

The incident beam at A is split by Bragg reflection in the first Si crystal plate[3] producing transmitted and reflected beams which are coherent. These are subsequently Bragg reflected in the middle crystal plate at points B and C. Two of the resulting beams are directed towards point D in the third crystal plate, where they mix and interfere. The outgoing beams entering the two He gas-filled proportional detectors C_2 and C_3 are linear combinations of the waves traversing paths ABD and ACD.

The transmitted and reflected waves in each plate get complex amplitudes, $a_t = t\ a_{in},\ a_r = r\ a_{in}$, with $t = \cos\phi$ and $r = i\sin\phi$, where the angle ϕ is real. Take the incoming wave at A to be[4] $\psi_0 = a_{in}e^{i\mathbf{k}_0\cdot\mathbf{r}}$ with $a_{in} = 1$ in arbitrary units, and set the origin of coordinates at point A. Label the paths ACD and ABD with the subscripts I and II respectively. Call L the side of the parallelogram $ABCD$. The parallelogram will be kept horizontal, $\varphi = 0$, in questions c.1-3 below.

c.1 (0.25 points) Write the waves at the input of the final plate, $\psi_{\text{I in}D}\,\psi_{\text{II in}D}$.

The wave along the path I has been transmitted in the first plate and then reflected towards D in the second; the wave along path II reflected twice. Thus,

$$\psi_{\text{I in}D} = r\ t\ e^{i2kL},\ \psi_{\text{II in}D} = r^2\ e^{i2kL},$$

where we neglected the small deflections and shifts in momentum along the paths worked out before, and used that the transmited $\mathbf{k}_0$ and reflected $\mathbf{k}_r$ momenta have the same magnitude k.

c.2 (0.25 points) Write out the waves ψ_2, ψ_3 **leaving the final plate towards the detectors** C_2 **and** C_3.

The wave ψ_2 is composed of parts coming from paths I and II that after arriving at D are transmitted and reflected towards detector C_2. Thus,

$$\psi_2(\mathbf{r}) = \left(t\ \psi_{\text{I in}D} + r\ \psi_{\text{II in}D}\right) e^{i\mathbf{k}_r\cdot(\mathbf{r}-\mathbf{r}_D)} = r(t^2 + r^2)\ e^{i(2kL + \mathbf{k}_r\cdot(\mathbf{r}-\mathbf{r}_D))}$$

Analogously, for the wave towards C_3

$$\psi_3(\mathbf{r}) = \left(r\ \psi_{\text{I in}D} + t\ \psi_{\text{II in}D}\right) e^{i\mathbf{k}_0\cdot(\mathbf{r}-\mathbf{r}_D)} = 2t\ r^2\ e^{i(2kL + \mathbf{k}_0\cdot(\mathbf{r}-\mathbf{r}_D))}$$

[3]The experiment uses Bragg reflection in the (220) lattice planes of the Si crystal. The Bragg angle is $\theta = 22.1^\circ$, the distance between plates $d = 3.5$ cm. Henceforth we neglect the thickness of the plates.

[4]From now on, use plane waves for the neutron wave function if you think it is reasonable.

Note that the transmitted wave vector is the incident one $\mathbf{k}_0 = k\hat{\mathbf{e}}_{in}$, while the reflected $\mathbf{k}_r = k\hat{\mathbf{e}}_r$makes an angle 2θ with $\mathbf{k}_0$. Detectors C_3 and C_2 are conveniently located in the path of these waves.

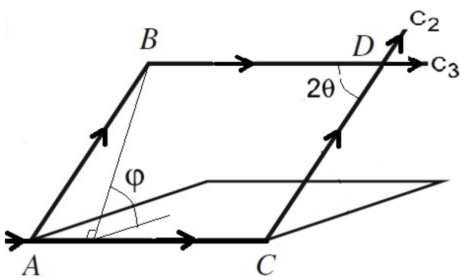
c.3 (0.5 points) Give the intensities I_2 and I_3 measured in the detectors in terms of the transmission and reflection coefficients T **and** R.

With $t^2 = |t|^2 = T$ and $l^2 = -|l|^2 = -R$, and $T + R = 1$, after some algebra

$$I_2 = |\psi_2|^2 = R - 4TR^2, \quad I_3 = |\psi_3|^2 = 4TR^2$$

Notice the destructive interference that occurs for a hypothetical 50/50 beam splitter, $\phi = \pi/2$, $\psi_2 = 0 = I_2$ and $I_3 = 1$.

The basic idea of the COW experiment is to tilt the interferometer about the incident beam line $\overline{AC}$ while maintaining the Bragg condition, causing a gravitationally-induced phase shift of the neutron deBroglie waves. So, the full parallelogram is in a tilted plane and the path $\overline{BD}$ is at a different height than $\overline{AC}$. Consider the case where the interferometer is rotated by an angle φ around $\overline{AC}$.



Tilted configuration by rotating the setup by an angle φ around the horizontal input direction $\overline{AC}$

The difference in the phases accumulated along path I and path II can be modified by varying the potential energy of the neutron along either of these two paths. These phase differences produce intensity swapping back and forth between the two detectors. Consider the case where the interferometer is rotated by and angle φ around $\overline{AC}$.

d. (1 point) Repeat[a] c.1-3, showing the emergence at D of a gravity-induced phase shift δ when the interferometer is tilted about the horizontal beam line $\overline{AC}$ by an angle φ. Calculateδ.

[a]Avoid calculating unnecesary integrals

We now have to consider the effect of gravity on the phases accumulated along paths I and II.

$$\psi_{\text{I in}D} = tre^{i(kL+\Phi_{CD})}, \quad \psi_{\text{II in}D} = r^2 e^{i(\Phi_{AB}+k_H L)}$$

Here, k and k_H are the wave numbers along the lower and upper paths $\overline{AC}$ and $\overline{BD}$ respectively, and $\Phi_{AB} = \Phi_{CD}$ the phases accumulated along $\overline{AB}$, $\overline{CD}$ (that we refrain from explicitly calculate). By energy conservation

$$p_H \approx p - \frac{m^2 gH}{p}, \quad \Rightarrow \quad k_H = k - 2\pi \frac{m^2 gH}{h^2}\lambda$$

where H is the height of $\overline{BD}$ over $\overline{AC}$ and λ the wavelength of the incident beam. Recalling that $\Phi_{AB} = \Phi_{CD}$we can write:

$$\begin{aligned}
\psi_2(\mathbf{r}_D) &= t^2 re^{i(kL+\Phi_{CD})} + r^3 e^{i(\Phi_{AB}+k_H L)} = re^{i(kL+\Phi_{CD})}\left\{t^2 + r^2 e^{i\delta}\right\} \\
\psi_3(\mathbf{r}_D) &= tr^2 e^{i(kL+\Phi_{CD})} + r^2 te^{i(\Phi_{AB}+k_H L)} = tr^2 e^{i(kL+\Phi_{CD})}\left\{1 + e^{i\delta}\right\}
\end{aligned}$$

where

$$\delta = (k_H - k)L = -2\pi \frac{m^2 gHL}{h^2}\lambda = -4\pi\lambda \frac{m^2 gd^2}{h^2}\tan\theta \sin\varphi$$

is the difference of phases accumulated along the horizontal paths $\overline{BD}$ and $\overline{AC}$.

The intensities I_2 and I_3 measured in the detectors can be written in the form:

$$I_2 = A - B(1+\cos\delta),\ I_3 = C(1+\cos\delta).$$

e. (1 point) Give A, B, and C in terms of T and R. Determine the number of fringes that will occur during a $180°$ rotation of the interferometer.

$$I_2 = |\psi_2|^2 = R - 2TR^2(1+\cos\delta);,\quad I_3 = |\psi_3|^2 = 2TR^2(1+\cos\delta)$$

Putting in the values of $m, g, \hbar$ and the parameters used in the COW experiment $\lambda = 1.445\text{Å}, \theta = 22.1°, d = 3.5$ cm gives[5]

$$\delta = 56.6\sin\varphi$$

The number of fringes during a rotation of 180° is

$$\Delta N_{180} = \frac{\delta(90°) - \delta(-90°)}{2\pi} = 18$$

During the experiment the interferometer was at rest in the laboratory frame and therefore rotating with the angular velocity of the Earth $\mathbf{\Omega}$.

f. (0.5 points) Write the momentum of the neutrons including the term due to the rotation of the reference frame of the interferometer.

Neutrons are rotating with respect to the center of the Earth's, therefore,

$$\mathbf{p} = m\mathbf{v} + m\,\mathbf{\Omega}\times(\mathbf{r}+\mathbf{R}),$$

where $\mathbf{r}$ and $\mathbf{v}$ are the neutron's position and velocity in the rotating frame of the interferometer, and $\mathbf{R}$ is the position of A with respect to the center of the Earth, which is independent of the neutron's instantaneous position.

The aditional term causes a phase shift δ_Ω to be added to δ calculated before.

g. (0.5 points) Show that δ_Ω can be written for any given orientation of the parallelogram using a surface integral S, yielding

$$\delta_\Omega = \frac{2m}{\hbar}\mathbf{\Omega}\cdot\mathbf{S}.$$

Indicate the direction of the vector S and give its value in terms of d and θ.

The additional momentum $\mathbf{p}_\Omega = m\,\mathbf{\Omega}\times(\mathbf{r}+\mathbf{R})$ generates the accumulation of different phases along paths I and II. This produces an additional phase shift:

$$\delta_\Omega = \Phi_{ACD} - \Phi_{ABD} = \frac{1}{\hbar}\int_{ACD}\mathbf{p}_\Omega\cdot d\mathbf{r} - \frac{1}{\hbar}\int_{ABD}\mathbf{p}_\Omega\cdot d\mathbf{r} = \frac{1}{\hbar}\oint_{ACDBA}\mathbf{p}_\Omega\cdot d\mathbf{r}$$

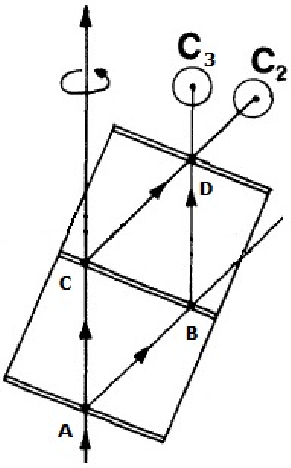
Now, using $(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c} = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$ and $\oint\mathbf{R}\times d\mathbf{r} = \mathbf{R}\times\oint d\mathbf{r} = 0$, we get

$$\delta_\Omega = \frac{m}{\hbar}\oint_{ACDBA}(\mathbf{\Omega}\times((\mathbf{r}+\mathbf{R}))\cdot d\mathbf{r} = \frac{m}{\hbar}\mathbf{\Omega}\cdot\oint_{ACDBA}\mathbf{r}\times d\mathbf{r} = \frac{2m}{\hbar}\mathbf{\Omega}\cdot\mathbf{S}.$$

The area vector $\vec{S}$ is orthogonal to the parallelogram $ABDC$, its direcction given by the corkscrew rule and its value is the parallelogram area $S = 2d^2\tan\theta$.

$$\Delta N_{\Omega,12°} = \frac{\delta_\Omega(\alpha=12°) - \delta_\Omega(\alpha=0°)}{2\pi} = \frac{4m}{h}\ \Omega S\ \cos\Phi\sin(12°)$$

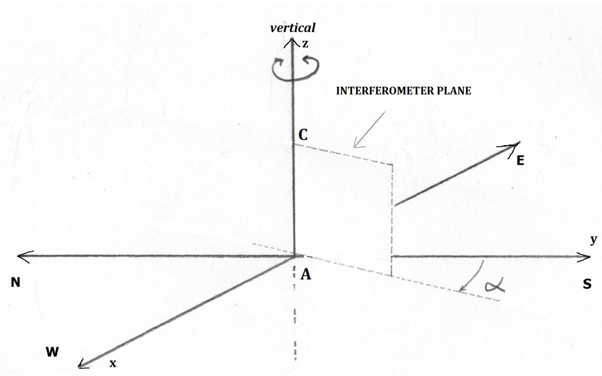
[5] There is a small discrepancy with the theoretical value given in the experiment since here we are neglecting the plate thickness.



Setup for question h. The interferometer rotates around the vertical direction $\overline{AC}$.

In an experiment, carried out in Columbia (Missouri, USA) at latitude $\Phi = 38.63°$ with an interferometer of area $S = 8.864$ cm^2 the incident beam was kept vertical.

h. (1 point) Determine the number of fringes registered in the detectors when the interferometer was initially set in the local meridian plane and was rotated 12° about the vertical direction $\overline{AC}$ from there.



The phase shift δ due to the gravitational field is independent of the orientation of the interferometer since it is kept in a vertical plane. In this configuration the vector $\mathbf{S}$ is orthogonal to the local vertical direction. In the coordinate system of the figure where yz is the local meridian plane, $\mathbf{S} = S(\cos\alpha, -\sin\alpha, 0)$ where α is the angle that S makes with the East-West direction, and $\mathbf{\Omega} = \Omega(0, \cos\Phi, \sin\Phi)$. Thus, $\mathbf{\Omega}\cdot\mathbf{S} = -\Omega S\cos\Phi\sin\alpha$, and

Numerically, $\frac{2m}{\hbar}\Omega S = 117.2$ deg, $\cos\Phi = \cos 38.63° = 0.7812 \Rightarrow \Delta N_{\Omega,12°} = 3.03$, i. e., three fringes.

Finally, you are asked to analyze how it is possible for waves incident on a crystal at a certain angle θ_B to emerge on the other side partly transmitted and partly reflected forming precisely an angle $2\theta_B$. Here we will study this phenomenon for neutron waves. The asymptotic form of the wave function at large distance r from the scattering center can be written in the Born approximation[6] as

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}_0\cdot\mathbf{r}} + f(\Delta\mathbf{k})\frac{e^{ikr}}{r}, \quad \text{where} \quad f(\Delta\mathbf{k}) = -\frac{m}{2\pi\hbar^2}\int d^3r' V(\mathbf{r}')e^{-i\Delta\mathbf{k}\cdot\mathbf{r}'},$$

where $|\mathbf{k}| = |\mathbf{k}_0| = k$. The goal here is to check if the sacttering amplitude $f(\Delta\mathbf{k})$ is only appreciable for momentum transfers $\Delta\mathbf{k} = \mathbf{k} - \mathbf{k}_0$, that fulfill the Bragg condition.

The atoms of the periodic crystal are located at $\mathbf{r}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_2\mathbf{a}_2$ with the n_i integers. The potential is periodic $V(\mathbf{r}_n + \mathbf{r}) = V(\mathbf{r})$ and, considering only the short range interactions of neutrons with the atomic nuclei of the crystal, it can be written as $V(\mathbf{r}) = \sum_n V\delta(\mathbf{r} - \mathbf{r}_n)$.

i. (1 point) Show that the scattering amplitude can be factored into an integral over the unit cell and a sum of phase factors. Use the notation $\mathbf{r} = \mathbf{r}_n + \mathbf{x}$ where $\mathbf{x}$ is a position within the unit lattice.

[6] This approximation underestimates the dynamics of the neutrons within the crystal as well as the finite size of the crystal.

$$f(\Delta\mathbf{k}) = -\frac{m}{2\pi\hbar^2}\int d^3r V(\mathbf{r})e^{-i\Delta\mathbf{k}\cdot\mathbf{r}} = -\frac{m}{2\pi\hbar^2}\sum_n \int_{\text{unit cell}} d^3x V(\mathbf{r}_n+\mathbf{x})\ e^{-i\Delta\mathbf{k}\cdot(\mathbf{r}_n+\mathbf{x})}$$
$$= \left(\sum_n e^{i\Delta\mathbf{k}\cdot\mathbf{r}_n}\right)\left(-\frac{m}{2\pi\hbar^2}\int_{\text{unit cell}} d^3x V(\mathbf{x})\ e^{-i\Delta\mathbf{k}\cdot\mathbf{x}}\right)$$

Where we first decomposed the integral into a sum of integrals over the cells and then used that $V(\mathbf{r}_n+\mathbf{x}) = V(\mathbf{x})$. The sum $\sum_n$ is a shorthand notation for $\sum_{(n_1,n_2,n_3)}$.

j. (1 point) Use the Poisson summation formula

$$\sum_{n=-\infty}^{+\infty} e^{ixan} = \frac{2\pi}{|a|}\sum_{m=-\infty}^{+\infty}\delta(x-\frac{2\pi}{a}m)$$

to show that in the limit of infinite number of scatterers $n_i \in (-\infty,+\infty)$ the scattering amplitude would be strictly zero for momentum transfers $\Delta\mathbf{k}$ that do not belong to the reciprocal lattice,

$$\Delta\mathbf{k}\cdot\mathbf{r}_n = \sum_n \Delta k_i\ a_i\ n_i, \quad \text{where} \quad \Delta k_i = \Delta\mathbf{k}\cdot\hat{\mathbf{a}}_i.$$

Thus,

$$\sum_{n_i} e^{i\Delta\mathbf{k}\cdot\mathbf{a}_i n_i} = \frac{2\pi}{|a_i|}\sum_{m=-\infty}^{+\infty}\delta(k_i-\frac{2\pi}{a_i}m)$$

Collecting the results for the three lattice vectors,

$$\left(\sum_n e^{i\Delta\mathbf{k}\cdot\mathbf{r}_n}\right) = \prod_{i=1}^{3}\left(\sum_{n_i} e^{i\Delta\mathbf{k}\cdot\mathbf{a}_i n_i}\right) = \frac{2\pi^3}{v}\sum_{m=-\infty}^{+\infty}\delta(\Delta\mathbf{k}-\mathbf{K}_m),$$

where $\mathbf{K}_m$, $m=(m_1,m_2,m_3)$ is a vector of the reciprocal lattice and v the volume of the unit cell.

k. (1 point) Use the above result to obtain the Bragg reflection formula.

We have $\mathbf{k}-\mathbf{k}_0 = \mathbf{K} \ \Rightarrow\ \frac{2\pi}{\lambda}(\hat{\mathbf{k}}-\hat{\mathbf{k}_0}) = \mathbf{K}$, also $\hat{\mathbf{k}}\cdot\hat{\mathbf{K}} = \sin\theta = -\hat{\mathbf{k}_0}\cdot\hat{\mathbf{K}}$, then

$$\frac{2\pi}{\lambda}\hat{\mathbf{K}}\cdot(\hat{\mathbf{k}}-\hat{\mathbf{k}_0}) = \hat{\mathbf{K}}\cdot\mathbf{K} \ \Rightarrow\ \frac{2\pi}{\lambda}2\sin\theta = |\mathbf{K}| \ \rightarrow 2\ d\ \sin\theta_B = n\ \lambda.$$

For simplicity, we wrote in the last term $d = 2\pi/|\mathbf{G}|$ where $\mathbf{G}$ is reciprocal lattice vector which corresponds to the family of lattice planes involved in the reflection. The factor n comes from simply considering $\mathbf{K} = n\mathbf{G}$.