
# Problems Booklet

Dear participants,

The PLANCKS 2025 exam is finally in your hands!

Below we remind you some of the most important rules of the contest

- The language used in the competition is English.
- The contest consists of 9 problems. Problems 1-8 each are worth 10 points, problem 9 is worth 15 points. Subdivisions of points are indicated in the problems.
- Each problem must be handed separately, i.e. no piece of paper should contain the resolution of more than one problem. Please mark the header of each sheet with your team name, the problem number, and the problem page number. It is necessary to mark each sheet so that it is scored.
- When a problem is unclear, a participant may request clarification through the invigilator. If the response is relevant to all teams, the jury will provide this information to the other teams.
- Participants are allowed to use a dictionary: English to your native language.
- Participants are allowed to use a non-programmable, not-graph calculator (scientific is okay).
- No books or other sources, except for this Problem Booklet and a dictionary, are to be consulted during the competition.
- The use of hardware (including phones, tablets etc.) is not approved, except for watches and medical equipment. Please leave your phones in an envelope.
- Participants may not leave the exam room until one hour after the start of the competition. Afterwards, they must obtain permission from the invigilator to use the restroom.
- The jury has the right to disqualify teams for misbehavior or breaking the rules.
- In situations to which no rule applies, the Organizing Committee decides.

We hope you enjoy solving these problems. Good luck and may the best team win!

*The Academic and Organizing Committees of* PLANCKS 2025

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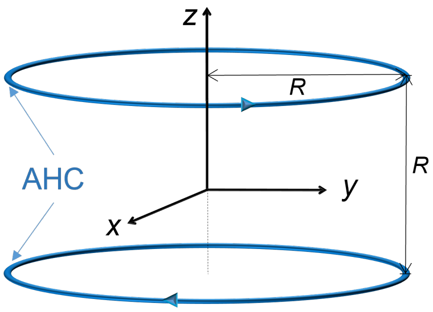
# PROBLEMS

# 1. Levitation in an Anti-Helmholtz coil

In some quantum magnetomechanical experiments a small magnetic particle is levitated in the magnetic field generated by two coaxial coils of the same radius $R$, separated by a distance $R$ (from center to center). The same current, $I$, circulates in the coils in opposite directions for each coil. This system is called an anti-Helmholtz coil (AHC). The origin of the coordinates is located at the geometric center of the AHC system (see figure).




1. [**5 points**] Evaluate the magnetic induction field, $\mathbf{B}_a$, (in Cartesian coordinates) created by the AHC at points close to the origin, $|\mathbf{r}| \ll R$, up to the first non-vanishing order in the different coordinates of $\mathbf{r}$.

2. Imagine a small sphere of radius $a$ ($a \ll R$) located at the origin of the coordinates. The sphere is made of linear, homogeneous, and isotropic (l.h.i) magnetic material characterized by magnetic susceptibility $\chi$. The position of the sphere can be perturbed with small displacements, $\vec{\varepsilon}$ ($|\vec{\varepsilon}| \ll R$). The sphere is small enough so that the field inside it can be considered uniform with the value at its center and its magnetization distribution, $\mathbf{M}$, is also uniform. For the sphere, the demagnetizing field is $\mathbf{H}_d = -(1/3)\mathbf{M}$. Disregard gravity.

   a. [**2.5 points**] Consider $\chi = -1$. Calculate the magnetic force over the sphere, $\mathbf{F}$, at the origin and study the stability of the system after small displacements, in terms of the stiffness coefficients, $\kappa_{\alpha\beta}$. The stiffness coefficients are defined as
   $$\kappa_{\alpha\beta} \equiv - \left. \frac{\partial F_\alpha}{\partial \beta} \right|_{\mathbf{r}=0},$$
   where $\alpha, \beta = (x, y, z)$.

   b. [**2.5 points**] Consider $\chi = +1$. Calculate the magnetic force over the sphere, $\mathbf{F}$, at the origin and study the stability of the system after small displacements, in terms of the stiffness coefficients, which are defined as before.

## Solution

Consider the $z$ axis as the coaxial axis of the system. The two coils of the AHC are located at $z_{1,2} = \pm R/2$. The induction field created by the AHC at any point of the $z$-axis is evaluated by the standard Biot-Savart law. The field of the coil at $z_1 = -R/2$ is

$$\mathbf{B}_1(\mathbf{r}) = \frac{\mu_0}{4\pi}\int_{c1} \frac{I\mathrm{d}\mathbf{l}_1 \times (\mathbf{r}-\mathbf{r}_1)}{|\mathbf{r}-\mathbf{r}_1|^3}, \tag{1}$$

where $\mu_0$ is the vacuum permeability. In our case $\mathbf{r}_1 = R\hat{\mathbf{u}}_\rho - (R/2)\hat{\mathbf{z}}$, $\mathbf{r} = z\hat{\mathbf{z}}$, $\mathrm{d}\mathbf{l}_1 = -IR\mathrm{d}\varphi\ \mathbf{u}_\varphi$. The only dependence on $\varphi$ appears in the unit vector $\hat{u}_\rho$, which, after the integral from 0 to $2\pi$ cancels. The induction field at a point on the $z$-axis becomes:

$$\mathbf{B}_1(z) = -\frac{\mu_0 I}{4\pi}\hat{\mathbf{z}}\int_{\varphi=0}^{2\pi}\frac{R^2}{\left[R^2+\left(z+\frac{R}{2}\right)^2\right]^{3/2}}\mathrm{d}\varphi = -\frac{\mu_0 I R^2}{2\left[R^2+\left(z+\frac{R}{2}\right)^2\right]^{3/2}}\hat{\mathbf{z}}. \tag{2}$$

Exactly in the same way but considering that the second coil is located at $z_2 = R/2$ and the $\mathrm{d}\mathbf{l}_2 = IR\mathrm{d}\varphi\ \hat{\mathbf{u}}_\varphi$, one gets:

$$\mathbf{B}_2(z) = \frac{\mu_0 I R^2}{2\left[R^2+\left(z-\frac{R}{2}\right)^2\right]^{3/2}}\hat{\mathbf{z}}. \tag{3}$$

Close to the origin, the sum of these expressions can be expanded, using the Taylor expansion, up to the first non-vanishing order in $z$. Thus, considering $|z| \ll R$, and using $(1+\epsilon)^{-3/2} \simeq 1-(3/2)\epsilon$ for $\epsilon \ll 1$, one gets

$$\mathbf{B}_\mathrm{a}(z) = \mathbf{B}_1(z) + \mathbf{B}_2(z) \simeq B_0\frac{2z}{R}\hat{\mathbf{z}}, \tag{4}$$

where we have defined $B_0 \equiv 24\mu_0 I/(25\sqrt{5}R)$, for convenience.
*[+1 point]*

This is the field along the $z$ axis. It has only a $z$-component. However, we want to obtain all the components of the induction field, evaluated at points $\mathbf{r}$ close to the origin ($|\mathbf{r}| \ll R$), but not necessarily on the axis. Using $\nabla\times\mathbf{B}_\mathrm{a} = 0$, and since $B_{\mathrm{a},x}$, $B_{\mathrm{a},y}$, $\frac{\partial B_{\mathrm{a},x}}{\partial z}$ and $\frac{\partial B_{\mathrm{a},y}}{\partial z}$ are zero at the axis, the $B_{\mathrm{a},z}$ component given in Eq. (4) is also valid, up to first order in $x$ and $y$, outside the axis because $\frac{\partial B_{\mathrm{a},z}}{\partial x} = \frac{\partial B_{\mathrm{a},z}}{\partial y} = 0$ . Moreover, the different components of the induction field will not depend on the *cross-coordinates*. That is, $B_{\mathrm{a},x}$ depends only on $x$ and $B_{\mathrm{a},y}$ only on $y$.
*[+2 points]*

Now, since $\nabla\cdot\mathbf{B}_\mathrm{a} = 0$, the induction field should satisfy:

$$\frac{\partial B_{\mathrm{a},x}}{\partial x} + \frac{\partial B_{\mathrm{a},y}}{\partial y} + \frac{\partial B_{\mathrm{a},z}}{\partial z} = 0. \tag{5}$$

Due to symmetry, $\frac{\partial B_x}{\partial x} = \frac{\partial B_y}{\partial y}$. Thus, Eq. (5) can be written as:

$$\frac{\partial B_x}{\partial x} = \frac{\partial B_y}{\partial y} = -\frac{1}{2}\frac{\partial B_z}{\partial z}. \tag{6}$$

With all this information and using Eqs. (4) and (6), the induction field components close to the origin are:

$$B_{\mathrm{a},x} = -B_0\frac{x}{R}, \tag{7}$$
$$B_{\mathrm{a},y} = -B_0\frac{y}{R}, \tag{8}$$
$$B_{\mathrm{a},z} = B_0\frac{2z}{R}. \tag{9}$$

Note the factor 2 and the different sign in the $z$-component. Expressed in vectorial form[1]:

$$\mathbf{B}_\mathrm{a}(\mathbf{r}) = B_0 \left( -\frac{x}{R}\hat{\mathbf{x}} - \frac{y}{R}\hat{\mathbf{y}} + \frac{2z}{R}\hat{\mathbf{z}} \right) = -B_0 \left( \frac{\mathbf{r} - 3z\hat{\mathbf{z}}}{R} \right). \tag{10}$$

*[+2 points]*

If we place a small sphere of radius $a$ close to the origin, this sphere will feel the applied field of the AHC. The small sphere is characterized by a constant susceptibility $\chi$. The sphere will magnetize. From the definition of susceptibility and demagnetizing field, $\mathbf{H}_d$, we can write:

$$\mathbf{M} = \chi\mathbf{H} = \chi(\mathbf{H}_a + \mathbf{H}_d) = \chi \left( \mathbf{H}_a - \frac{1}{3}\mathbf{M} \right), \tag{11}$$

where $\mathbf{H}$ is the magnetic field inside the sphere, $\mathbf{H}_a$ is the magnetic field created by the AHC ($\mathbf{H}_a = \mathbf{B}_a/\mu_0$). The magnetization can be written in terms of the susceptibility and the applied induction field[2]:

$$\mathbf{M} = \frac{3\chi}{\mu_0(3+\chi)}\mathbf{B}_a. \tag{12}$$

As the sphere is assumed small ($a \ll R$), its magnetization can be assumed uniform inside it. The applied field considered is the one at the center of the sphere. Thus, the sphere can be considered as a small magnetic dipole whose magnetic moment $\mathbf{m}$ equals $\mathbf{m} = V\mathbf{M}$, where $V$ is the volume of the small sphere [$V = (4/3)\pi a^3$].
*[+2 points]*

The magnetic force acting over a dipole, due to an externally applied field is known to be:

$$\mathbf{F} = (\mathbf{m} \cdot \nabla)\mathbf{B}_a. \tag{13}$$

In the present case, one has

$$\mathbf{F} = \left( V \frac{3\chi}{\mu_0(3+\chi)}\mathbf{B}_a \cdot \nabla \right) \mathbf{B}_a. \tag{14}$$

Using the equations of the $\mathbf{B}_a$ [Eq. (10)], simple algebra allows us to evaluate the force and, from it and using the definitions given, the stiffness coefficients (written in matrix form):

$$\mathbf{F} = \frac{4\pi a^3}{3\mu_0} \left( \frac{3\chi}{3+\chi} \right) \frac{B_0^2}{R} \left( \frac{x}{R}\hat{\mathbf{x}} + \frac{y}{R}\hat{\mathbf{y}} + \frac{4z}{R}\hat{\mathbf{z}} \right), \tag{15}$$

$$\kappa = -\frac{4\pi a^3}{3\mu_0} \frac{B_0^2}{R^2} \left( \frac{3\chi}{3+\chi} \right) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 4 \end{pmatrix}. \tag{16}$$

Note that the factor $\frac{3\chi}{3+\chi}$ is equal to $-3/2$ and $3/4$, for $\chi = -1$ and $\chi = +1$, respectively. Thus, for $\chi = -1$ and $\chi = +1$, the forces are

$$\mathbf{F}_{\chi=-1} = \frac{4\pi a^3}{3\mu_0} \left( -\frac{3}{2} \right) \frac{B_0^2}{R} \left( \frac{x}{R}\hat{\mathbf{x}} + \frac{y}{R}\hat{\mathbf{y}} + \frac{4z}{R}\hat{\mathbf{z}} \right), \tag{17}$$

$$\mathbf{F}_{\chi=+1} = \frac{4\pi a^3}{3\mu_0} \left( \frac{3}{4} \right) \frac{B_0^2}{R} \left( \frac{x}{R}\hat{\mathbf{x}} + \frac{y}{R}\hat{\mathbf{y}} + \frac{4z}{R}\hat{\mathbf{z}} \right). \tag{18}$$

The force is zero when the sphere is exactly at the center of the AHC (when $x = y = z = 0$). This indicates that the center of the AHC is an equilibrium position. However, after small perturbations, the forces are different from

[1] It is not necessary to know it, but this is the expression of a quadrupolar field.

[2] The problem can be solved directly by substituting the values of $\chi$ but we go on here using general expressions, to facilitate the final interpretation of the results

zero. To evaluate the stability of this equilibrium position, we evaluate the stiffness coefficients. A positive stiffness will indicate a restoring force after a perturbation (stable equilibrium). For $\chi = -1$ and $\chi = +1$ one gets

$$\kappa_{\chi=-1} = \frac{4\pi a^3}{3\mu_0}\left(\frac{3}{2}\right)\frac{B_0^2}{R^2}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 4\end{pmatrix}, \tag{19}$$

$$\kappa_{\chi=+1} = -\frac{4\pi a^3}{3\mu_0}\left(\frac{3}{4}\right)\frac{B_0^2}{R^2}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 4\end{pmatrix}. \tag{20}$$

*[+1.5 points]*

In the case $\chi = -1$, all stiffness coefficients are positive, indicating that the sphere is stably levitating in the center of the AHC as any perturbation will be counteracted with a restoring force. Note also that the stability is stronger against perturbations along the $z$ direction than in the $x$ or $y$ direction. When $\chi = +1$, all the stiffness coefficients are negative, indicating that the center of the AHC is an unstable equilibrium position for the sphere. In fact, it is unstable against perturbations in any direction.
*[+1.5 points]*

To add some information, it is easily seen from Eq. (16) that the $\mathbf{r} = 0$ equilibrium position is stable for $\chi < 0$ spheres (diamagnetic spheres), whilst the system is unstable for $\chi > 0$ ones (paramagnetic spheres). The case $\chi = -1$ would correspond to a perfect diamagnetic sphere (a superconducting one in the Meissner state) with $\mathbf{B} = 0$ inside it. The case $\chi \to \infty$ would correspond to an ideal soft ferromagnetic sphere where $\mathbf{H} = 0$ in its interior. The case $\chi = 0$ corresponds to a non-magnetic sphere ($\mathbf{M} = 0$) and, obviously, it will feel no force coming from the AHC magnetic induction field, independently of its position.

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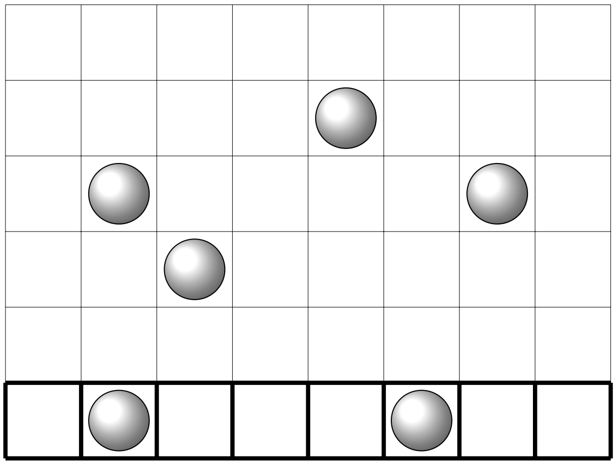
## 2. Surface Adsorption




Gas adsorption on solid surfaces has a significant impact on the design of advanced materials for many applications. For instance, materials such as MOFs (Metal-Organic Frameworks) are actively studied to capture $CO_2$ or hydrogen, of great interest in environmental science and energy storage. In this problem, we will explore a simple model of gas adsorption on a surface.

Let us consider a gas confined in a container and study the adsorption of particles at the walls. We will study the process by neglecting the kinetic energy of the particles and using a discrete model for the locations of the particles in the bulk and on the surface (see figure). Let $N_B$ be the number of possible spatial cells the particles may occupy in the bulk and $N_S$ be the number of spatial cells on the surface. The gas consists of $N$ particles and $N_B \geq N \geq N_S$. Let $n$ be the number of particles actually on the surface: $0 < n \leq N_S$. A particle has an energy $-\epsilon$ (binding energy) while it is on the surface and 0 while it is in the bulk. $N_B$, $N_S$ and $N$ are all constants and very large; $n$ is a variable and also large. The volume of a gas cell is $V_0$.

1. [**2 points**] Using the microcanonical ensemble find the entropy as a function of $n$. Make use of the Stirling approximation.

2. [**2 points**] Derive an expression relating $n$ to the temperature of the system. Find the limit of $n/N$ when $T \to \infty$ and $T = 0$ reasoning your results.

3. [**2 points**] Derive the expression for $n = n(T)$ but now using the canonical ensemble. Compare your result with that derived in question (2) and reason your results.

4. [**2 points**] Assume $N_B \gg N \gg N_S$. Find the explicit relation $n = n(T)$. For which temperature value a surface cell is equally likely to be occupied or unoccupied?

5. [**2 points**] In the limit $N_B \gg N \gg N_S$, find the fraction of adsorbed particles $\theta \equiv n/N_S$ in terms of the gas pressure and plot $\theta$ vs $p$ for a fixed temperature (this is named Langmuir isotherm). Find the pressure for which half of the particles are adsorbed. Give a physical interpretation of the dependence of $\theta$ with $p$.

## Solution

1. Each microstate for the particles in the bulk is defined by the number of empty cells and occupied cells, $n_e$ and $n_o$ respectively. Since $n$ is the actual number of particles on the surface, the number of microstates of the bulk $\Omega_B$ is the number of ways of placing $N-n$ particles in $M_B$ bulk cells, with $n_o = N-n$ and $n_e = N_B - (N-n)$, so that

$$\Omega_B = \frac{(n_o+n_e)!}{n_o!n_e!} = \frac{N_B!}{(N-n)!(N_B-N+n)!}.$$

Analogously, for the particles in the surface, since $n_o = n$ and $n_e = N_s - n$, one finds

$$\Omega_S = \frac{N_S!}{n!(N_s-n)!}.$$

The entropy follows from the Boltzmann formula $S = k_B \ln \Omega$ where $\Omega = \Omega_B \Omega_S$. Hence,

$$\begin{aligned} S &\simeq k_B \left[ N_B \ln\left(\frac{N_B}{N_B-N+n}\right) + (N-n)\ln\left(\frac{N_B-N+n}{N-n}\right) + N_S \ln\left(\frac{N_S}{N_S-n}\right) \right. \\ &+ \left. n\ln\left(\frac{N_S-n}{n}\right)\right], \end{aligned}$$

making use of the Stirling approximation.

2. The energy of the system is $E = -n\epsilon$ and the temperature

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_N = \frac{\partial S}{\partial n}\frac{\partial n}{\partial E} = -\frac{1}{\epsilon}\frac{\partial S}{\partial n} = -\frac{k_B}{\epsilon}\ln\left[\frac{(N-n)(N_S-n)}{n(N_B-N+n)}\right]$$

so that

$$\frac{(N-n)(N_S-n)}{n(N_B-N+n)} = e^{-\frac{\epsilon}{k_BT}}.$$

When $T\to\infty$ one has $e^{-\frac{\epsilon}{k_BT}} \simeq 1$, so that $(N-n)(N_S-n) = n(N_B-N+n)$ and finally

$$\frac{n}{N} = \frac{N_S}{N_S+N_B}.$$

In the high temperature limit the binding energy is negligible and the fractional occupation of surface cells is identical to the fractional occupation of all the cells. As $T\to 0$ one has $e^{-\frac{\epsilon}{k_BT}} \simeq 0$ and so $n = N_S$, which corresponds to the minimum energy of the system.

3. A possible way to obtain $n(T)$ using the canonical ensemble is to deal the bulk and the surface separately and find the chemical potentials. Finally, $n(T)$ may be found when bulk and surface reach equilibrium, i.e., when both chemical potentials are equal.

For the particles in the bulk, each microstate has energy 0 so that, denoting $n_g$ the number of particles in the gas, the partition function is

$$Z_B = \sum_s e^{-\beta E_s} = \Omega_B = \frac{N_B!}{n_g!(N_B-n_g)!}$$

while for the particle in the surface, since each microstate has energy $-n\epsilon$, one finds

$$Z_S = \Omega_S e^{\beta n\epsilon} = \frac{N_S!}{n!(N_s-n)!}e^{\beta n\epsilon}.$$

The system is in equilibrium when the chemical potential of the particles in the bulk equals the chemical potential of the particles in the surface. The chemical potential can be found from the partition function. Thus,

$$\mu_B = k_BT\frac{\partial \ln Z_B}{\partial n_g} \simeq k_BT\ln\left(\frac{N_B-n_g}{n_g}\right) = k_BT\ln\left(\frac{N_B-N+n}{N-n}\right)$$

with $n_g = N - n$. Analogously,

$$\mu_S = k_B T \frac{\partial \ln Z_S}{\partial n} \simeq \epsilon + k_B T \ln\left(\frac{N_S - n}{n}\right).$$

Finally, equating the chemical potentials one recovers the equation

$$\frac{(N-n)(N_S-n)}{n(N_B - N + n)} = e^{-\frac{\epsilon}{k_B T}}.$$

This result is expected since this equation is also the state equation for the energy (recall that $E = -n\epsilon$) of the system in terms of the energy and the state equations can be derived from any ensemble.

4. For $N_B \gg N \gg N_S$ one can consider the approximations $N - n \simeq N$ and $N_B - N + n \simeq N_B$. Then,

$$\frac{n}{N_S} \simeq \frac{1}{\frac{N_B}{N} e^{-\frac{\epsilon}{k_B T}} + 1}.$$

The occupation probability of the cells in the surface is the fraction of particles in the surface: $n/N_S$. For this probability to be 1/2, $n/N_S = 1/2$ so that $\frac{N_B}{N} e^{-\frac{\epsilon}{k_B T}} \simeq 1$. Finally,

$$T \simeq \frac{\epsilon}{k_B \ln(N_B/N)}.$$

5. The gas pressure can be calculated using the expression for $Z_B$ above

$$p = -\left(\frac{\partial F}{\partial V}\right)_{n_g, T} = \frac{k_B T}{V_0}\left(\frac{\partial \ln Z_B}{\partial N_B}\right)_{n_g, T} = -\frac{k_B T}{V_0} \ln(1 - n_g/N_B) \simeq \frac{NkT}{V}$$

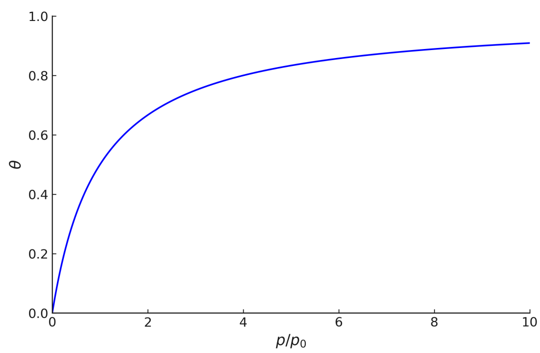
where we have used Stirling approximation and that $n_g = N - n \simeq N$ in the limit $N_B \gg N \gg N_S$. This is the ideal gas equation.

By substituting $N = pV/k_B T$ in the expression for $\frac{n}{N_S}$ found in question 4 one obtains

$$\theta = \frac{n}{N_S} = \frac{1}{\frac{N_B K_B T}{pV} e^{-\frac{\epsilon}{k_B T}} + 1} = \frac{p}{p + p_0}$$

with $p_0 = \frac{k_B T}{V_0} e^{-\frac{\epsilon}{k_B T}}$.

This is precisely the pressure for which the surface is half covered. When $p$ is small the amount of gas particles is small and then few particles get absorbed in the surface. As $p$ is large enough (much larger than $p_0$), there are many particles in the gas, the flux of gas particles onto the surface is large and most surface sites are occupied.

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# 3. Second sound

Heat transport in semiconductors is essential in many areas of nanotechnology. For instance, the rate at which heat is evacuated in nanocircuits determines the actual limits for the speed of computation in what is called the “thermal wall”. In bulk materials, heat transport is usually described by Fourier’s law, and it is said to be diffusive. Things work differently when the system length or time scales are comparable to the mean free path or mean free times of heat carriers. Here we will study the possibility of heat waves, what is known as second sound. It was first observed in the 70’s at cryogenic temperatures for just a few materials, and recently in graphite and in germanium at larger temperatures. To this end, we consider the so-called Maxwell-Cattaneo equation for the heat flux $\mathbf{q}$

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -\kappa \nabla T, \tag{1}$$

with $T$ the temperature, $\kappa$ the thermal conductivity and $\tau$ the heat flux relaxation time, which in semiconductors is an average mean free time for phonon resistive scattering.

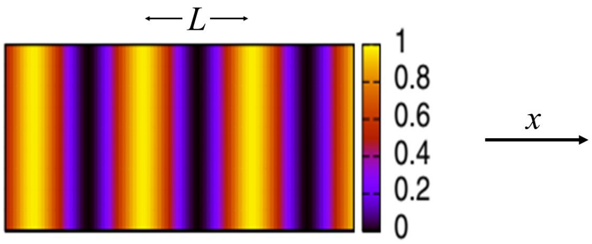
In what follows, assume the Maxwell-Cattaneo equation and that volume does not change.

## Questions

1. [**1 point**] Show that in some limit one recovers Fourier’s law.

2. [**2 points**] Show that in some limit the temperature propagates as a wave, and that the speed of this wave is smaller than (first) sound speed. Hint: consider that the thermal conductivity is $\kappa = \frac{1}{3} C_V c^2 \tau$, with $C_V$ the heat capacity per unit volume and $c$ the speed of sound; this expression can be obtained at low enough temperatures for three dimensional materials assuming Debye model with identical branches.

One type of experiment to detect the wave-like behaviour of temperature is by instantaneously heating the surface of the dielectric with a laser with a spatially periodic pulse of period $L$, providing an initial perturbation $\Delta T(x, 0) = A\cos(2\pi x/L)$ (see figure), and measure how the system relaxes to equilibrium (these are called thermal grating experiments). Let us assume that heat flows only in the $x$ axis.




3. [**3 points**] Find the evolution of the induced temperature difference $\Delta T(x, t)$ and the range of $L$ for which one could observe at least one temperature oscillation before reaching equilibrium.

4. [**1 point**] Discuss the possibility of finding that heat flows from cold to hot.

5. [**3 points**] Let us now analyze the compatibility of the Maxwell-Cattaneo equation (1) with the second law of thermodynamics. Find the entropy production assuming local-equilibrium and discuss its sign. Do the same if one assumes a non-equilibrium entropy density of the type

$$s(u, \mathbf{q}) = s_{eq}(u) - \frac{\tau}{2\kappa T^2}\mathbf{q}^2,$$

where $u$ is the energy density and $s_{eq}$ the local-equilibrium entropy density.

Note: neglect terms higher than quadratic in the entropy production.

## Solution

1. If the time scale of the experiment is $t_p$ one can estimate the order of magnitude of the derivative of **q** in (1) as

$$\tau \frac{\partial \mathbf{q}}{\partial t} \approx \frac{\tau}{t_p} \mathbf{q}$$

Then, if the time scale of the experiment is much larger than $\tau$, $t_p \gg \tau$, one can neglect the derivative as compared to the **q** term in (1) and recover Fourier's law, $\mathbf{q} = -\kappa \nabla T$.

2. In order to obtain an equation for the temperature, we must combine Eq. (1) with the equation for energy conservation. Since volume is constant, $du = C_V dT$, with $C_V$ the heat capacity per unit volume, and one has

$$C_V \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0, \tag{2}$$

which yields

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \frac{\kappa}{C_V} \nabla^2 T. \tag{3}$$

For perturbations much shorter than $\tau$ (or for frequencies $\omega >> \tau^{-1}$), the term in the second time derivative is much greater than the one in the first time derivative so that we are left to the wave equation.

The speed of this wave (second sound), with the help of $\kappa = \frac{1}{3} C_V c^2 \tau$, is

$$v_{SS}^2 = \frac{\kappa}{C_V \tau} = \frac{c^2}{3}$$

Then $v_{SS} = c/\sqrt{3} < c$.

*Historical note:* Eq. (3) is the so-called Telegrapher's equation, first derived by Heaviside to describe transmission lines in 1876. Let us recall its technological and economic importance after the first transoceanic line. Heaviside, who was a telegrapher, was who wrote Maxwell's equations as we know them (and specified that they should be called Maxwell's equations), and applied them to obtain the Telegrapher's equation (for voltage). Lord Kelvin also made important contributions to the topic from a different perspective.

3. In order to find the evolution of the temperature difference $\Delta T(x,t)$ one solves Eq. (3) trying a solution of the type

$$\Delta T(x,t) \propto \exp(i\omega t)\cos(kx),$$

with $k \equiv 2\pi/L$, which supplies

$$\tau\omega^2 - i\omega = \frac{\kappa}{C_V} k^2 \ \Rightarrow$$

$$\omega = \frac{1}{2\tau}\left(i \pm \sqrt{\frac{4\kappa\tau}{C_V}k^2 - 1}\right)$$

Then, if the term inside the square root is negative, $\omega$ is purely complex with positive imaginary parts, $\omega_\pm = i|\omega_\pm|$, so that $\Delta T(x,t)$ decays exponentially, i.e. there is no oscillation. However, if the term inside the square root is positive, $\omega$ has a real part, i.e. $\omega = \omega_r + i/2\tau$. Then the solution reads

$$\Delta T(x,t) = A\exp(-\frac{t}{2\tau})\cos(\omega_r t)\cos(2\pi x/L),$$

with $\omega_r = \sqrt{\frac{4\kappa\tau}{C_V}k^2 - 1}/2\tau$. This corresponds to a damped oscillation, i.e. a decaying standing wave. Accordingly, oscillations could be seen provided that the period $L$ is short enough.

In order to observe an oscillation, this must occur before it has died out. Then, the period of the oscillation must be shorter than the time scale of decay, which is $2\tau$ ($4\tau$ would also be ok), i.e.

$$\frac{2\pi}{\omega_r} < 2\tau.$$

This yields

$$L < \frac{2\pi}{\sqrt{1+4\pi^2}}\sqrt{\frac{\kappa\tau}{C_V}} \simeq v_{SS}\,\tau.$$

4. The Maxwell-Cattaneo equation (1) allows heat to flow from cold to hot if $\tau\frac{\partial \mathbf{q}}{\partial t}$ is large enough and has the appropriate sign. One situation where this becomes apparent is for the standing waves studied above. After half a period, a cold region becomes hotter than its surroundings. Then, heat has flown from cold to hot.

   Another way of proving that the heat flux in a wave is opposite to the thermal gradient at some instants is by using the energy conservation equation (2). Let us consider the limit where one has a true wave equation (with no damping). The wave solution is $T, \mathbf{q} \propto \exp i(kx - \omega t)$, with $k$ and $\omega$ real numbers. Eq. (2) supplies

   $$C_V \omega T = kq$$

   i.e. $\mathbf{q}$ is in phase with $T$, and then it is $\pi/2$ out of phase with $\nabla T$. As a result, half of the time the heat flux is opposite to the thermal gradient.

5. The second law of thermodynamics states that the entropy production $\sigma_s \geq 0$. It can be obtained from the balance equation for entropy

   $$\frac{ds}{dt} + \nabla\cdot\mathbf{J_s} = \sigma_\mathbf{s}, \tag{4}$$

   with $s$ the entropy per unit volume and $\mathbf{J_s} = \mathbf{q}/\mathbf{T}$ the entropy flux.

   i) Assuming the local-equilibrium hypothesis, the entropy density is that of equilibrium in a local version:

   $$ds_{eq} = T^{-1}du,$$

   with $u$ the internal energy density (let us recall that volume is constant). By using the energy conservation equation, one has

   $$\sigma_s = T^{-1}\frac{du}{dt} + \nabla\cdot\frac{\mathbf{q}}{T} = -T^{-1}\nabla\cdot\mathbf{q} + \nabla\cdot\frac{\mathbf{q}}{T} = -\frac{\mathbf{q}\cdot\nabla T}{T^2}.$$

   For Fourier's law, the latter expression can be written as

   $$\sigma_s = \frac{\mathbf{q}^2}{\kappa T^2} > 0,$$

   but for Maxwell-Cattaneo reads

   $$\sigma_s = \frac{\mathbf{q}^2 + \tau\,\mathbf{q}\cdot\frac{d\mathbf{q}}{dt}}{\kappa T^2},$$

   which has no definite sign. Then it might violate the second law of thermodynamics.

   ii) However, assuming a non-equilibrium entropy which depends on the equilibrium variable $u$ and the nonequilibrium variable $\mathbf{q}$ of the type

   $$s(u,\mathbf{q}) = s_{eq}(u) - \frac{\tau}{2\kappa T^2}\mathbf{q}^2$$

   one has

   $$ds = T^{-1}du - \frac{\tau}{\kappa T^2}\mathbf{q}\cdot d\mathbf{q},$$

   and

   $$\sigma_s = T^{-1}\frac{du}{dt} - \frac{\tau}{\kappa T^2}\mathbf{q}\cdot\frac{d\mathbf{q}}{dt} + \nabla\cdot\frac{\mathbf{q}}{T} = -\frac{\mathbf{q}}{T^2}\cdot\left(\nabla T + \frac{\tau}{\kappa}\frac{d\mathbf{q}}{dt}\right),$$

which for Maxwell-Cattaneo writes

$$\sigma_s = \frac{\mathbf{q}^2}{\kappa T^2} > 0.$$

In summary, the Maxwell-Cattaneo equation (1) does not violate the second law of thermodynamics, but it requires to introduce a nonequilibrium entropy beyond the local-equilibrium hypothesis.

As a final comment, thermal waves is an example of hydrodynamic transport, a hot topic of research which includes thermal and electronic transport and exhibits other interesting phenomena.

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# 4. Some questions about our universe

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• Answer the questions in a clear, structured and concise manner, underlining the final result.
• Before starting to solve the problems, read the Formulae section on the next page, where you will find some useful equations and definitions that you need.

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1.a. [**1 point**] Assume a component of the universe $A$ having an equation of state relating pressure and energy density of the form $P_A = w_A\, \rho_A$, with constant $w_A$. Use the Friedmann eqs in the Formulae to show that the behaviour of $\rho_A$ with respect the scale factor $a$ is of the form

$$\rho_A \propto a^{\pi_A}$$

and calculate $\pi_A$ as a function of $w_A$.

1.b. [**1 point**] The dependence of the energy density on $a$ can be deduced from physical arguments in the case of $A = M, R, \Lambda$. (i) For matter, $\rho_M \propto a^{-3}$ because of dilution due the expansion of the universe, (ii) for radiation, $\rho_R \propto a^{-4}$ because in addition of dilution we have energy redshift, and (iii) for the cosmological constant, the energy density $\rho_\Lambda$ is constant (independent of $a$).

Use the facts (i), (ii) and (iii) and what you got in **(a)** to deduce the values of $w_M$, $w_R$, $w_\Lambda$.

*(FYI: The form of $\rho_M(a)$, $\rho_R(a)$, and $\rho_\Lambda(a)$ allows to catch some properties of the evolution of the universe.)*

2.a. [**2 points**] **(a)** From the Friedmann eqs shown in Formulae one can find an equation giving $\ddot{a}(t)$

$$\ddot{a} = aG\,(\alpha\rho + \beta P)$$

($\rho$ = total energy density, $P$ = total pressure). Calculate the value of the constants $\alpha$ and $\beta$.

2.b. [**2 points**] Define the deceleration parameter $q_0$

$$q_0 = -\left.\frac{a\ddot{a}}{\dot{a}^2}\right|_0$$

where $a, \dot{a}$ and $\ddot{a}$ are taken at $t = t_0$ (today's time).

Calculate $q_0$ as a function of $\Omega_M$, $\Omega_R$ and $\Omega_\Lambda$ (and nothing else).

*(FYI: In our universe $\Omega_\Lambda$ dominates, leading to $q_0 < 0$, i.e. now the universe is accelerating)*

3. Consider a flat universe ($k = 0$) with matter and cosmological constant ($\rho_R = 0$). The objective is to calculate the age of such an universe $t_0$.

   a. [**2 points**] Show that $t_0$ is given by an integral

   $$t_0 = \int_{\alpha_1}^{\alpha_2} da\, f(a, H_0, \Omega_M, \Omega_\Lambda)$$

   Find the values of integral limits $\alpha_1$ and $\alpha_2$. Find the function $f$.

   b. [**2 points**] Solve the integral, and find $t_0$ as a analytical function that depends only on $H_0$ and on $\Omega_\Lambda$. (You will need several substitutions, you might start with $x = a^{3/2}$)

*(FYI: With the observed values of $H_0$ and $\Omega_\Lambda$ we get the age of our universe, to a very good approximation.)*

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### Formulae

We denote by $a = a(t)$ the scale factor of the universe (we will normalize $a(t_0) = 1$) and by $H = H(t) = \dot{a}/a$ the Hubble parameter (function of time $t$), and the Hubble constant by $H_0 = H(t_0)$. The time $t_0$ is today's time. As usual $\dot{a} = da/dt$ and $\ddot{a} = d^2a/dt^2$.

The total energy density of the universe is given by the sum of all contributions $\rho = \sum_A \rho_A$ and similarly for the total pressure, $P = \sum_A P_A$. The first and second Friedmann equations are

$$\text{1st eq:} \qquad H^2 = \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\,\rho - \frac{k}{a^2} \qquad \text{2nd eq:} \qquad \frac{d\rho_A}{dt} = -\,3H\,(\rho_A + P_A)$$

($G$ = Newton's const., $k$ =curvature of the universe). Note that the 2nd eq is actually an equation for each $A$. Summing over $A$ we get $d\rho/dt = -\,3H\,(\rho + P)$.

We define the critical density $\rho_c$ and the quantities $\Omega_A$

$$\rho_c = \frac{3H_0^2}{8\pi G}\,, \qquad \Omega_A \equiv \frac{\rho_A(t_0)}{\rho_c}$$

In the problem that we propose, we consider 3 (ideal) fluid components in the universe: matter ($M$), radiation ($R$), and cosmological constant ($\Lambda$). ($M$ is non relativistic matter and $R$ are photons or similar.) In these cases, the relation between energy density and pressure (equation of state) is linear: $P_A = w_A\,\rho_A$, with $w_M = 0$, $w_R = 1/3$, $w_\Lambda = -1$. Finally, we have $\Omega_M = \rho_M(t_0)/\rho_c$, and similarly for $R$ and $\Lambda$.

## Solution

**1.)** (a) The 2n Friedmann eq (together with $P_A = w_A \, \rho_A$) gives

$$\frac{d\rho_A}{\rho_A} = -3(1 + w_A)\,\frac{da}{a} \implies \rho_A \propto a^{-3(1+w_A)}$$

Therefore $\pi_A = -3(1 + w_A)$

(b) Taking into account the information I give in (i), (ii), and (iii), clearly $w_M = 0$, $w_R = 1/3$, $w_\Lambda = -1$

**2.)** (a) Take the time-derivative of 1st Friedmann eq and substitute $d\rho/dt = -\,3H\,(\rho + P)$ where $\rho$ and $P$ are the total energy density and total pressure. Get

$$2\dot{a}\ddot{a}/a^2 - 2\dot{a}^3/a^3 = -8\pi G(\dot{a}/a)(\rho + P) + 2k\dot{a}/a^3$$

All terms have a factor $H$, simplify the expression and, finally, use again 1st Friedmann eq to get

$$\frac{\ddot{a}}{a} = -\,\frac{4\pi G}{3}\,(\rho + 3P)$$

Therefore

$$\alpha = -\,4\pi/3. \qquad \beta = -\,4\pi$$

(b)

$$q_0 = \frac{4\pi G}{3H_0^2}\;(\rho + 3P)|_0 = \frac{1}{2\rho_c}\,(\rho_0 + 3P_0) = \frac{1}{2}\sum(1 + 3w_A)\,\Omega_A$$

Thus

$$q_0 = \frac{1}{2}\Omega_M + \Omega_R - \Omega_\Lambda$$

**3.)** (a) From the definition of $H(t)$

$$dt = \frac{1}{H}\,\frac{da}{a}$$

For a flat universe with matter and cosmological constant we have $k = 0$ and the Friedmann eq can be written in the form $H = H_0\sqrt{\Omega_M/a^3 + \Omega_\Lambda}$. Thus

$$t_0 = \frac{1}{H_0}\int_0^1 \frac{da/a}{\sqrt{\Omega_M/a^3 + \Omega_\Lambda}}$$

(b) The integral can be solved with different substitutions. For example

$$\int \frac{a^{1/2}da}{\sqrt{\Omega_M + \Omega_\Lambda a^3}} = \int \frac{2}{3}\frac{dx}{\sqrt{\Omega_M + \Omega_\Lambda x^2}} = \int \frac{2}{3\sqrt{\Omega_\Lambda}}\frac{dy}{\sqrt{1 + y^2}} = \int \frac{2}{3\sqrt{\Omega_\Lambda}}dz = \frac{2}{3\sqrt{\Omega_\Lambda}}z$$

where we use the substituions $x = a^{3/2}$, $\;y = \sqrt{\Omega_\Lambda/\Omega_M}\,x$, $\;z = \sinh^{-1} y$.

Final answer (we use $\Omega_M + \Omega_\Lambda = 1$ to eliminate $\Omega_M$ as required)

$$t_0 = \frac{2}{3H_0\sqrt{\Omega_\Lambda}}\;\sinh^{-1}\left(\sqrt{\frac{\Omega_\Lambda}{1 - \Omega_\Lambda}}\right)$$

An alternative way to solve $\int dy/\sqrt{1 + y^2}$ is with the substitution $y = \tan\theta$,

$$\int \frac{dy}{\sqrt{1 + y^2}} = \int d\theta\,\sec\theta = \ln|\sec\theta + \tan\theta| = \ln|\sqrt{1 + y^2} + y|$$

Then we get

$$t_0 = \frac{2}{3H_0\sqrt{\Omega_\Lambda}}\;\ln\left(\frac{\sqrt{\Omega_\Lambda} + 1}{\sqrt{1 - \Omega_\Lambda}}\right)$$

The two results for $t_0$ are identical.

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# 5. Black Hole Shadow

We would like to observe the "shadow" of a black hole with an earth-based telescope system. To do so, we consider a Schwarzschild black hole around which matter orbits at radii ranging from the innermost stable circular orbit (ISCO) until larger distances. That matter will emit light, which we want to picture with our telescopes. Note: In this exercise we do not consider bending of light rays in the vicinity of the black hole.

1. In order to calculate the radius of the ISCO, we consider the effective potential energy given by General Relativity (GR) for a test mass $m$, located at distance $r$ from the black hole center and angular momentum $L$:

$$V_{\text{eff}}(r) = -\frac{GmM}{r} + \frac{L^2}{2mr^2} - \frac{R_s}{2} \cdot \frac{L^2}{mr^3}, \tag{1}$$

where $G$ is the gravitational constant, $M$ the mass of the black hole, $R_s = 2\,GM/c^2$ the Schwarzschild radius and $c$ the light speed.

   a. [**1.5 points**] Find the effective potential energy for Newton's law of gravitation in terms of the angular momentum and compare with the GR one. In which situations the GR effects will be relevant and in which not?

   From now on consider Eq. (1) and that $L$ is a constant of motion.

   b. [**1 point**] Find the orbits $r = r(L)$ and show that there exists a minimum value of $L$.

   c. [**4 points**] Find the range of possible orbits $r$, the range of $r$ for stable solutions and the ISCO radius. Hint: you may find helpful to plot $L^2$ vs $r$, but it is not mandatory to reach the maximum mark.

2. A relatively close and active supermassive black hole in the vicinity of our Galaxy has a mass of approximately $5 \times 10^9 M_\odot$ (where the solar mass $M_\odot = 2 \times 10^{30}$ kg), and a distance of 16.7 Mpc (1 pc = $3.1 \times 10^{16}$ m).

   a. [**0.5 points**] Calculate the angular extension of the ISCO radius of that supermassive black hole, if observed from Earth.

   b. [**3 points**] To picture that black hole, we need to design a system that reaches an angular resolution better than the angular extension of the object derived in the previous section, in the best case at least twice as good. The best angular resolutions can be achieved through interferometric observations, where the same incident wave is detected by pairs of distant telescopes, and their signals get multiplied by each other to generate an interference pattern (in the so-called correlator). The angular resolution is then approximately $\lambda/D$, where $\lambda$ denotes the wavelength of the observed light wave and the $D$ the distance between a telescope pair. At large distances, both telescopes can only register the signals, digitize them and correlate them later offline. Technically, delay precisions between different stations of the order to $\sim 1$ ps are feasible... (continued on the next page)...

The following picture shows the transparency of the terrestrial atmosphere to light at different wavelengths. Can you choose a suitable observation wavelength for the interferometer and the required minimum distance between two telescope pairs to achieve the angular resolutions found in question 2a?

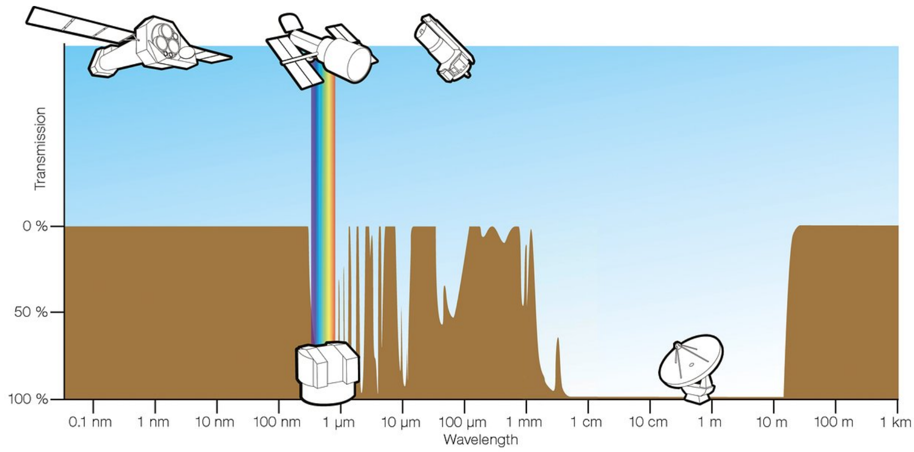


Figure 1: Transparency of the Earth's atmosphere. Note the <u>inverted</u> vertical scale. Credit: ESA/Hubble (F. Granato).

Constants: $G = 6.7 \times 10^{-11} \mathrm{m}^3\,\mathrm{kg}^{-1}\mathrm{s}^{-2}$; $c = 3 \times 10^8\,\mathrm{m/s}$; Earth radius= $6378\,\mathrm{km}$.

## Solution

**1.)** (a) Considering Newton's law of gravitation, the mechanical energy of a test mass $m$ in a circular orbit around a star is the sum of potential and kinetic energy

$$-\frac{GmM}{r} + \frac{1}{2}mv^2 = -\frac{GmM}{r} + \frac{L^2}{2mr^2},$$

since in classical mechanics $L = mrv$. Comparing the latter expression with Eq. (1) one finds that GR introduces a new term, the last one in the right-hand-side, which is an attractive term. Comparing the second and third terms in (1) one finds that the latter can be neglected as compared to the second one when $R_s \ll r$, i.e. far away form the black hole, but it is relevant when $r$ is comparable to $R_s$.

(b) We calculate the first derivative of the effective potential energy and set it to zero to find an extreme (considering constant $L$)

$$\frac{\partial V_{\text{eff}}(r)}{\partial r} \stackrel{!}{=} 0 = \frac{GmM}{r^2} - \frac{L^2}{mr^3} + \frac{3R_s}{2} \cdot \frac{L^2}{mr^4} \tag{2}$$

The first equation has the following two solutions:

$$r = \frac{L^2 \pm \sqrt{L^4 - 12L^2G^2M^2m^2/c^2}}{2GMm^2} \quad . \tag{3}$$

We note that for $r$ to be a real number, the lowest possible angular moment is $L = \sqrt{12}GMm/c = \sqrt{3}\, mR_s c$. Notice that this contrasts to Newtonian mechanics, where there is no intrinsic minimum value of $L$.

(c) In the previous question we have found two possible solutions for the orbits radii, one for each sign before the square root. Since $r_+$ is a growing function of $L$, it moves between $r(L_{min}) = 6GM/c^2 = 3R_s$ to infinity when $L \to \infty$. The interval corresponding to the $r_-$ solution is more involved to calculate but it can be seen to range in the interval $1.5R_s < r < 3R_s$. Then the range of orbit solutions of Eq. (1) is $r > 1.5\, R_s$. To study the stability of the solutions one must verify that $V_{\text{eff}}$ is a minimum. To achieve this, one evaluates the second derivative of $V_{\text{eff}}$,

$$\frac{\partial^2 V_{\text{eff}}(r)}{\partial r^2} = -\frac{2GmM}{r^3} + \frac{3L^2}{mr^4} - 6R_s \cdot \frac{L^2}{mr^5}. \tag{4}$$

Isolating $GmM$ from Eq. (2) one finds

$$\frac{\partial^2 V_{\text{eff}}(r)}{\partial r^2} = \frac{L^2}{mr^5}\left(r - 3R_s\right),$$

so that $r_-$ are unstable solutions and $r_+$ are stable ones. Therefore the radius of the ISCO is $r_{\text{ISCO}} = 3R_s$.

An alternative way of answering these questions is expressing the orbits equation $L^2$ as a function of $r$. Eq. (2) yields

$$L^2 = GMm^2\frac{r^2}{r - 3/2R_s}, \tag{5}$$

which provides positive physical solutions for the range $r > 3/2\, R_s$. When $r \to 3/2\, R_s$ and when $r \to \infty$ one has $L \to \infty$, so that there is a minimum in between (see fig. 2).
Differentiating Eq. (5)

$$\frac{dL^2}{dr} = GMm^2\frac{r^2 - 3R_s r}{(r - 3/2R_s)^2},$$

one finds the orbit for $L_{min}$ to be $3\, R_s$, as found in (b).

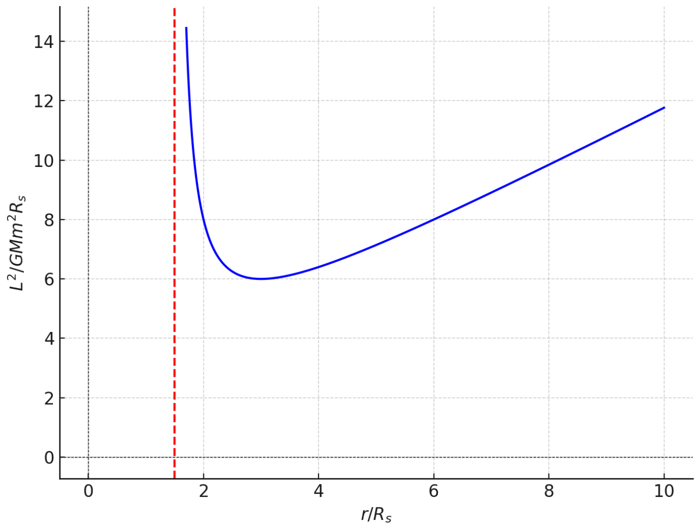


Figure 2: Plot of scaled $L^2$ vs $r$, showing a minimum.

Again, for each value of $L$ we find two solutions, one at each side of the minimum. To check the stability one employs the second derivative, Eq. (4). Substituting $L^2$ from (5) one finds

$$\frac{\partial^2 V_{\text{eff}}(r)}{\partial r^2} = \frac{GmM}{r^3}\frac{r-3R_s}{r-3/2R_s},$$

so that the solutions $3/2\,R_s < r < 3R_s$ are unstable and the solutions $r > 3R_s$ are stable. Accordingly,

$$r_{\text{ISCO}} = 3R_s \tag{6}$$

as found before.

**2.)** (a) First, we calculate the extension of the ISCO. Inserting the numbers into Eq. 6, we obtain $r_{\text{ISCO}} = 4.5 \times 10^{13}$ m. The angular size $\theta$ of an object of the size of $r_{\text{ISCO}}$ located at $16.7 \times 10^6$ pc from Earth is then (1 pc = $3.1 \times 10^{16} m$) :

$$\theta = \arctan\frac{r_{\text{ISCO}}}{D_{\text{BH}}} \approx \frac{r_{\text{ISCO}}}{D_{\text{BH}}} = 8.6 \times 10^{-11}\ \text{rad} \tag{7}$$

Note that the angular extension of the ISCO is actually twice that value.

(b) Delay precisions of the order $\varDelta = 1$ ps lead to a limiting accuracy of the phase measurement of $\varDelta\phi/2\pi \approx \frac{c\cdot\varDelta}{\lambda}$. The chosen wavelength should hence be at least several times $c\varDelta = 300\,\mu$m, which excludes the infrared part of the spectrum. The next suitable atmospheric transparency window lies at around 0.9 mm. For this wavelength and the required angular resolution of, say, half the ISCO diameter, a baseline of $D = \frac{\lambda}{\theta} = 1 \times 10^7$ m is needed, about 80% of the Earth's diameter. Possible solutions from 1 mm to 1.3 mm are also allowed, but note that if the wavelength is taken larger than 1.4 mm, baselines longer than the Earth's diameter are required, and the answer is therefore not correct.

Finally, let us comment that these telescopes must be placed on mountains, the higher the better; in the case of ALMA (Atacama Large Millimeter Array) they are located at more than 5000 m altitude), because the opacity of the atmosphere is already quite important at wavelengths below 1 mm.

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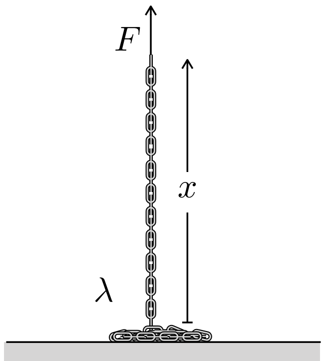
# 6. Pulling a chain upwards with constant force

Consider pulling one end of a very long chain initially piled up on a table with a constant force $F$, as illustrated in the figure. At the start, a very short segment of length $x_0$ is held vertically at rest. The chain is subject to Earth's gravitational attraction, with a constant acceleration $g$.
The chain consists of links that are infinitesimally small in both length and mass, allowing it to be treated as a continuous system with a uniform linear mass density $\lambda$. Neglect the height and horizontal spread of the pile on the table.




1. [**3 points**] Derive the ordinary differential equation for the velocity $v$ of the rising segment of a chain as a function of its height $x$ (1 point), and solve it to obtain the expression (2 points)

$$v = \sqrt{\frac{F}{\lambda}\left(1 - \frac{x_0^2}{x^2}\right) - \frac{2}{3} g x_0 \left(\frac{x}{x_0} - \frac{x_0^2}{x^2}\right)}$$

   *Hint:* You may need an integrating factor $\mu(x)$ to solve the equation.

2. [**1 point**] Determine the maximum height $x_{\max}$ of the chain that can be reached with the applied force.

3. [**1 point**] Explain why $x_{\max}$ exceeds the equilibrium height $x_{\text{eq}} = F/(\lambda g)$, where the force $F$ balances the chain's weight.

In the remaining sections, assume that the initial height $x_0$, where pulling begins, is much smaller than the equilibrium height, i.e., $x_0 \ll x_{\text{eq}}$.

4. [**1 point**] Determine $x(t)$ for timescales much larger than $x_0\sqrt{\lambda/F}$ and up to the moment when the end of the chain reaches its maximum height.

5. [**2 points**] Obtain the velocity of the descending segment of the chain as a function of $x$ after the chain has reached its maximum height $x_{\max}$.

6. [**1 point**] Calculate the minimum height, $x_{\min}$, that the vertical segment of the chain will reach during its descent.

   *Hint:* The equation

$$\frac{3}{2} - \xi + \log\left(\frac{2\xi}{3}\right) = 0$$

   has two solutions, $\xi_0 = 3/2$ and $\xi_1 \approx 0.625$.

7. [**1 point**] Sketch an approximate graph of $x(t)$ for a time interval that includes several cycles as described in the previous questions.

## Solution

**1.)** Consider the variable-mass system consisting of the segment of the chain that is not in contact with the ground. In this case, Newton's second law/general mass accretion formula is expressed as:

$$F - (\lambda x)g = \frac{d}{dt}\left[(\lambda x)\dot{x}\right],$$

where $\lambda x$ represents the mass of the system. Expanding this equation gives:

$$F - \lambda g x = \lambda \dot{x}^2 + \lambda x \ddot{x}.$$

Next, we use the well known relation $\ddot{x} = v dv/dx = (1/2)d(v^2)/dx$, where $v = \dot{x}$. Substituting this into the previous equation, we obtain:

$$2\frac{F}{\lambda} - 2gx = 2v^2 + x\frac{dv^2}{dx}.$$

The integrating factor for this ODE is $x$, which allows us to rewrite the equation as:

$$2x\frac{F}{\lambda} - 2gx^2 = 2xv^2 + x^2\frac{dv^2}{dx} = \frac{d}{dx}\left(x^2v^2\right).$$

Now, integrating both sides with respect to $x$, we find:

$$\frac{F}{\lambda}(x^2 - x_0^2) - \frac{2}{3}g(x^3 - x_0^3) = x^2v^2.$$

Finally, solving for $v$, we get:

$$\boxed{v = \sqrt{\frac{F}{\lambda}\left(1 - \frac{x_0^2}{x^2}\right) - \frac{2}{3}gx_0\left(\frac{x}{x_0} - \frac{x_0^2}{x^2}\right)}} \tag{1}$$

**2.)** To find $x_{\max}$, we set $v^2 = 0$. To simplify the derivation, we introduce the dimensionless variable $\zeta := x_{\max}/x_0$:

$$0 = \frac{F}{\lambda}\left(\zeta^2 - 1\right) - \frac{2}{3}gx_0\left(\zeta^3 - 1\right) = (\zeta - 1)\left[\frac{F}{\lambda}(\zeta + 1) - \frac{2}{3}gx_0\left(\zeta^2 + \zeta + 1\right)\right].$$

This equation simplifies to

$$\frac{2}{3}gx_0\zeta^2 + \left(\frac{2}{3}gx_0 - \frac{F}{\lambda}\right)\zeta + \left(\frac{2}{3}gx_0 - \frac{F}{\lambda}\right) = 0,$$

which has the solution

$$x_{\max} = x_0\zeta = \frac{\sqrt{\left(\frac{F}{\lambda} - \frac{2}{3}gx_0\right)\left(\frac{F}{\lambda} + 2gx_0\right)} + \frac{F}{\lambda} - \frac{2}{3}gx_0}{\frac{4}{3}g}.$$

Note that the second root of the quadratic equation is not physical, as it would correspond to negative values for $x_{\max}$. Finally,

$$\boxed{x_{\max} = \frac{\sqrt{3\left(3F - 2gx_0\lambda\right)\left(F + 2gx_0\lambda\right)} + 3F - 2gx_0\lambda}{4g\lambda}}$$

**3.)** There is no contradiction. For $x < x_{\text{eq}}$, the constant force $F$ exceeds the force required for equilibrium, providing a net upward velocity at the moment when $x = x_{\text{eq}}$. This propels the vertical section of the chain beyond $x_{\text{eq}}$.

**4.)** For these timescales we have $x_0/x = o(1)$ and equation (1) can be simplified (taking the limit $x_0 \to 0$) as:

$$v = \sqrt{\frac{F}{\lambda} - \frac{2}{3}gx}.$$

In this case, we obtain the following approximation:

$$t = \int_0^x \frac{dx'}{v} = \int_0^x \frac{dx'}{\sqrt{\frac{F}{\lambda} - \frac{2}{3}gx'}} = -\frac{3}{g}\sqrt{\frac{F}{\lambda} - \frac{2}{3}gx'}\Bigg|_0^x = \frac{3}{g}\left(\sqrt{\frac{F}{\lambda}} - \sqrt{\frac{F}{\lambda} - \frac{2}{3}gx}\right).$$

Solving for $x$, we find:

$$x = \frac{3}{2g}\left[\frac{F}{\lambda} - \left(\sqrt{\frac{F}{\lambda}} - \frac{gt}{3}\right)^2\right].$$

Finally:

$$\boxed{x = t\left(\sqrt{\frac{F}{\lambda}} - \frac{1}{6}gt\right), \qquad t \gg x_0\sqrt{\frac{F}{\lambda}}}$$

**5.)** The descending motion of the chain is governed by:

$$F - (\lambda x)g + \dot{x}\frac{d}{dt}(\lambda x) = \frac{d}{dt}\left[(\lambda x)\dot{x}\right].$$

The third term on the left-hand side arises because an additional force is exerted by the table on the bottommost link of the suspended segment of the chain to halt its motion. Alternatively, this result can be derived from the general mass accretion formula, with the term accounting for the fact that when the bottommost link loses contact with its upper neighbors before being brought to rest by the table, its velocity matches that of the falling segment. The above formula simplifies to

$$F - (\lambda x)g = (\lambda x)\ddot{x}.$$

Using again $\ddot{x} = v dv/dx = (1/2)d(v^2)/dx$, where $v = \dot{x}$ we have

$$\frac{F}{\lambda x} - g = v\frac{dv}{dx} = \frac{1}{2}\frac{d(v^2)}{dx}.$$

From which we obtain, after taking into account the initial condition $v = 0$ at $x = x_{\max}$,

$$\boxed{v = \sqrt{2g(x_{\max} - x) - \frac{2F}{\lambda}\log\left(\frac{x_{\max}}{x}\right)}}$$

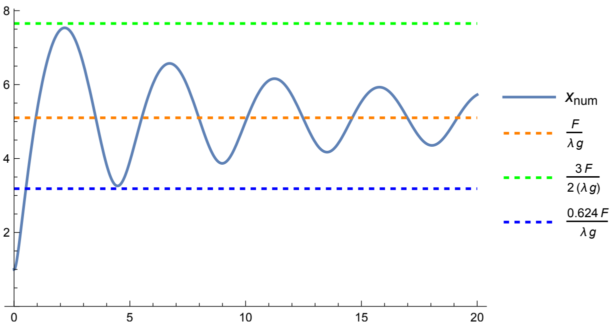
**6.)** The minimum height is obtain by equating the velocity to zero. If we write $x$ as $x = (F/\lambda g)\xi$ and recall that $x_{\max} = 3F/(2\lambda g)$, we have the equation

$$0 = \frac{\lambda}{2F}v^2 = \frac{\lambda g}{F}(x_{\max} - x) - \log\left(\frac{x_{\max}}{x}\right) = \frac{3}{2} - \xi - \log\left(\frac{3}{2\xi}\right).$$

Hence, using the hint,

$$\boxed{x_{\min} = \frac{F}{\lambda g}\xi_1 = 0.625\frac{F}{\lambda g}}$$

**7.)** The plot you are asked to provide should have the following appearance:

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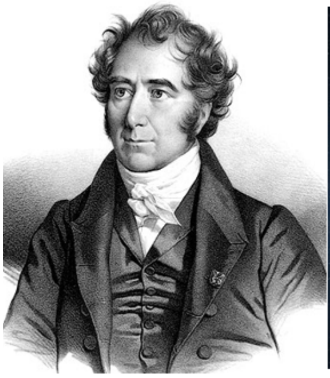
# 7. Stellar observation: from diffraction to interferometry




In 1818, Augustin-Jean Fresnel presented his work on the wave theory of light in front of the French Academy of Sciences. The panel included eminent scientists of the time, such as Simèon Denis Poisson and François Arago. Fresnel argued that light behaved as a wave, contrary to Newton's corpuscular theory, which still had many followers.

During the presentation, Poisson, a staunch supporter of the corpuscular theory, argued that if Fresnel's wave theory were correct, a bright spot should be observed at the centre of the shadow cast by an opaque circular object, which seemed absurd. However, Arago decided to test this prediction. To the surprise of many, the experiment confirmed the existence of this bright spot, now known as Poisson's spot or Arago's spot. This result provided strong evidence in favour of the wave theory of light, marking a milestone in the history of optics.

Many years have passed since Arago conducted his famous experiment, and in that time, humanity has achieved incredible feats, such as sending telescopes into space that bring us closer to the deepest mysteries of the universe. However, what Fresnel and his colleagues discovered remains vitally important today. Their work not only revolutionized our understanding of light but also laid the foundation for the development of advanced optical technologies. Today, the diffraction phenomenon they studied is fundamental to understanding the resolving power of optical instruments like the James Webb Space Telescope, allowing us to explore the cosmos with unprecedented clarity.

## Questions

Suppose Arago conducts a second experiment where he illuminates an opaque square object, with side length $l$, using coherent light (both spatially and temporally) emitted by an oil lamp with a central wavelength $\lambda_c$. The light source is placed at a sufficiently large distance from the object to consider that it is illuminated with plane waves.

1. [**3 points**] Applying the Fraunhofer approximation, calculate the intensity distribution (diffraction pattern) as a function of the position $x$ and $y$ on the screen if it is located at a distance $D \gg l$, and the angular position of the first diffraction minimum in direction $x$ and direction $y$. Is there a bright spot?

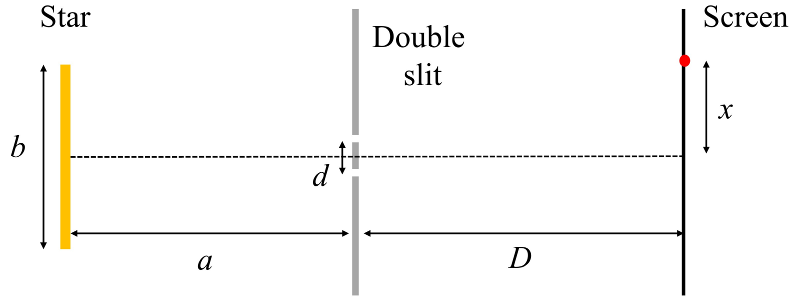
2. Let us now assume an astronomical telescope with a square aperture of side length $L$:

   a. [**1 point**] Write the equation for the angular resolving power of this telescope using Rayleigh's criterion. Justify your answer.

   b. [**1 point**] Determine if this telescope can resolve as separate objects the binary star system of Sirius, composed of Sirius A and Sirius B, with an angular distance of approximately $\theta = 10$ arc seconds. Note: Assume that Sirius A and B present the same energy flux at the telescope plane, that we are observing in the visible range with an average wavelength of $\lambda = 550$ nm. The telescope's square aperture has a side length of $L = 2.4$ meters. (Note: $1^\circ = 3600$ arc seconds).

3. [**3 points**] Now we move the telescope to observe the Orion constellation. We set up a double slit (Young's double slit) attached to the telescope objective to implement a Michelson stellar interferometer (see the figure below for reference). Let us consider the one-dimensional model depicted in the figure, where $b$ is the size of a star, $d$ the distance between slits, $a$ is the distance of the star to the telescope, and $D$ the distance of the slits

to the screen ($a, D \gg d$). Assuming that the intensity emitted by the star is uniform, calculate the visibility function, $V = \frac{I_{max}-I_{min}}{I_{max}+I_{min}}$. (Note: $\sin A - \sin B = 2 \sin \frac{A-B}{2} \cos \frac{A+B}{2}$). Neglect the diffraction effects of the aperture.




4. [**2 points**] When Michelson used the stellar interferometer to study the star Betelgeuse, a red giant star located in the Orion constellation, he found that the first minimum of visibility of the interference fringes occurred at a distance between the slits of $d$ = 308 cm. Using an average wavelength of 570 nm, what is the angular diameter of the star? If the distance to Orion is estimated to be 1.6 $10^{15}$ km, what is the diameter of the star?

## Solution

**1.)** The framework of Fraunhofer diffraction, the complex amplitude at the propagated far field, corresponding to an object distribution given by $U(\xi, \eta)$ can be calculated as,

$$U(x,y) = \left(\frac{\exp(ikz)}{i\lambda z}\right) \exp\left(\frac{i\pi}{\lambda z}(x^2+y^2)\right) \iint U(\xi,\eta) \exp\left(-\frac{i2\pi}{\lambda z}(\xi x + \eta y)\right) d\xi d\eta \tag{1}$$

where $(\xi, \eta)$ are the coordinates at the object plane and $(x, y)$ are the coordinates at the propagated plane, and with $\lambda$, $z$, and $k$ being the wavelength, propagated distance, and wavenumber, respectively.

Under this scenario, if we calculate the diffraction for a squared aperture of size $L$, we obtain:

$$U(x,y)\Big|_{\text{square}} = \alpha \iint_{-L/2}^{L/2} U_0 \exp\left(-\frac{i2\pi}{\lambda D}(x\xi + y\eta)\right) d\xi d\eta = U_0 \alpha L^2 \left(\frac{\sin\left(\frac{\pi x L}{\lambda D}\right)}{\frac{\pi x L}{\lambda D}}\right) \left(\frac{\sin\left(\frac{\pi y L}{\lambda D}\right)}{\frac{\pi y L}{\lambda D}}\right) \tag{2}$$

where we have rewritten $\alpha = \left(\frac{\exp(ikz)}{i\lambda z}\right) \exp\left(\frac{i\pi}{\lambda z}(x^2+y^2)\right)$ for simplicity and with $U_0$ being the amplitude distribution at the object which is considered constant over the whole aperture.

Since the intensity is proportional to the square of the amplitude, the intensity distribution at the far field can be written as,

$$I(x,y)\Big|_{\text{square}} \propto I_0 \left(\frac{\sin\left(\frac{\pi x L}{\lambda D}\right)}{\frac{\pi x L}{\lambda D}}\right)^2 \left(\frac{\sin\left(\frac{\pi y L}{\lambda D}\right)}{\frac{\pi y L}{\lambda D}}\right)^2 \tag{3}$$

with $I_0 = \left(\frac{U_0 L^2}{\lambda D}\right)^2$ and where we have set the distance between the object and the screen to $z = D$.

At this stage, we can calculate the first minimum of the obtained intensity distribution in Eq. (3). For the $x$ direction it is obtained when the $\sin\left(\frac{2\pi x L}{\lambda D 2}\right)^2 = 0$, which leads to,

$$\theta_{\text{min,x}} \approx \frac{x}{D} = \frac{\lambda}{L} \tag{4}$$

Analogously for the $y$ direction: $\theta_{\text{min,y}} \approx \frac{y}{D} = \frac{\lambda}{L}$. In relation to the existence of a bright spot with the rectangular geometry, the answer is yes: equation (3) provides a maximum at $x = y = 0$. The minima calculated above give the size of this spot.

However, at this point, we must take into account that we do not have a square aperture, but rather a solid opaque square object of the same dimension. Note that if we have a complex plane wave and we calculate the Fraunhofer diffraction, the transform will take the form,

$$\int_{-\infty}^{+\infty} \exp(iu\xi)\, d\xi = 2\pi\delta(u) \tag{5}$$

where $\delta(u)$ represents the Dirac delta function evaluated at the spatial frequencies $u$.

This integral can be decomposed as the sum of two terms:

$$\int_{-\infty}^{\infty} \dots dx = \left( \int_{-\infty}^{-L/2} \dots dx + \int_{L/2}^{\infty} \dots dx \right) + \int_{-L/2}^{L/2} \dots dx \tag{6}$$

The term in parentheses corresponds to the diffraction of an obstruction, while the last integral corresponds to the diffraction of an aperture. Thus, the amplitude distribution of the obstruction and the aperture are equal and of opposite sign, except at the origin, so the intensity distribution will be the same, except at the origin. This implies that the position of the minima will be the same, so the result obtained in Eq. (4) is valid for the opaque square. This result is in agreement with Babinet's principle.

**2.)** (a) The Rayleigh criterion states that two points are resolvable when the central maximum of one diffraction pattern coincides with the first minimum of the other. In our case, since the objective aperture is square, the diffraction pattern will correspond to that found in section 1, and the angular distance to the first minimum will give the angular resolution power. Therefore, the angular resolution power is given by Eq. (4).

(b) On the one hand, the angular separation of $S_A$ and $S_B$ in radians will be,

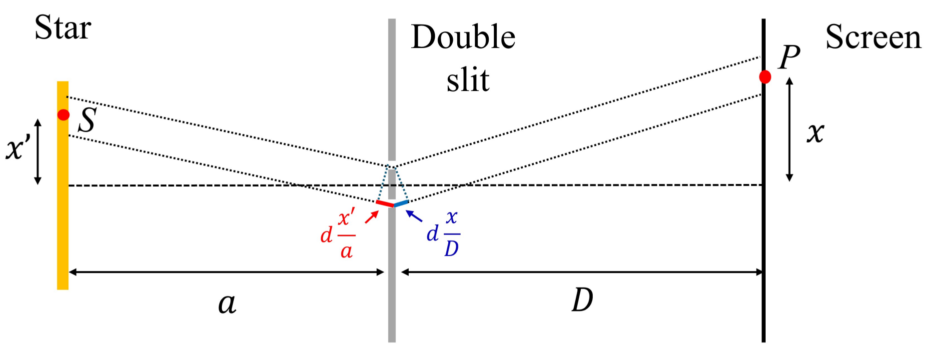
$$\Delta\theta = 10'' \times \frac{1^\circ}{3600''} \times \frac{\pi\,\text{rad}}{180^\circ} = 4.8 \times 10^{-5}\,\text{rad} \tag{7}$$

On the other hand, the angular resolution power of the telescope will be,

$$\theta_{\text{RP}} = \frac{\lambda}{L} = \frac{550 \times 10^{-9}\,\text{m}}{2.4\,\text{m}} = 2.3 \times 10^{-7}\,\text{rad} \tag{8}$$

So, as $\Delta\theta > \theta_{\text{RP}}$, we can resolve.

**3.)** The interference scheme is the following:




Since $a, D \gg d$, the path difference between two rays that leave point $S$ and arrive at point $P$, is

$$\Delta = x\frac{d}{D} + x'\frac{d}{a}. \tag{9}$$

And the retardance is

$$\delta(x, x') = \frac{2\pi}{\lambda}\Delta = \frac{2\pi}{\lambda}\left(x\frac{d}{D} + x'\frac{d}{a}\right) \tag{10}$$

Considering Eq. (10), the intensity per unit length at point $P$ on the screen, due solely to the contribution from point $S$ of the source, can be found from the general interference equation,

$$\frac{I(x,x')}{b} = \frac{2I_0}{b}\left(1+\cos\delta(x,x')\right) = \frac{2I_0}{b}\left(1+\cos\left(\frac{2\pi d}{\lambda}\left(\frac{x}{D}+\frac{x'}{a}\right)\right)\right) \tag{11}$$

where $b$ is the star diameter and where we have assumed that the intensity coming from the two slits is the same.

Total intensity is found by integrating Eq. (11) over all source differentials,

$$I = \int_{-b/2}^{b/2} \frac{I(x,x')}{b}\,dx' = 2I_0\left[1+\frac{\sin\left(\frac{\pi bd}{a\lambda}\right)}{\frac{\pi bd}{a\lambda}}\cos\left(\frac{2\pi x}{\Delta x}\right)\right] \tag{12}$$

with $\Delta x = \frac{\lambda D}{d}$.

Recall the expression for visibility,

$$V = \frac{I_{\text{max}} - I_{\text{min}}}{I_{\text{max}} + I_{\text{min}}} \tag{13}$$

where in our case, $I_{\text{max}}$ and $I_{\text{min}}$ are the maxima and minima intensity from Eq. (12).

Considering maxima and minima intensities occurring with $\cos\left(\frac{2\pi x}{\Delta x}\right) = \pm 1$, they take the explicit expression:

$$I_{\text{max}} = 2I_0\left[1+\frac{\sin\left(\frac{\pi bd}{a\lambda}\right)}{\frac{\pi bd}{a\lambda}}\right], \qquad I_{\text{min}} = 2I_0\left[1-\frac{\sin\left(\frac{\pi bd}{a\lambda}\right)}{\frac{\pi bd}{a\lambda}}\right] \tag{14}$$

Replacing Eqs. (14) in Eq. (13), the visibility can be written as:

$$V = \frac{\sin\left(\frac{\pi bd}{a\lambda}\right)}{\frac{\pi bd}{a\lambda}} \tag{15}$$

**4.)** The statement tells us that when Michelson used the stellar interferometer to study the star Betelgeuse, he found that the first minimum of visibility of the interference pattern occurred for a distance between the slits $d = 308$ cm. Considering the relationship we found for visibility, Eq. (15), for this particular value of the distance between slits, it must be satisfied that $V = 0$, this leading to,

$$\frac{b}{a} = \frac{\lambda}{d} \tag{16}$$

where we have set the condition of first minimum ($m = 1$).

On the other hand, we can find a relationship for the angular diameter of the star Betelgeuse, geometrically, this leading to:

$$\theta \approx \frac{b}{a} \tag{17}$$

where we have approximated the tangent directly to the angle because the star is far away ($a = 1.6 \times 10^{18}$m) from the earth, and thus, the angular angle is very small.

With Eqs. (16) and (17), and substituting the known values, we obtain,

$$\theta = \frac{\lambda}{d} = \frac{570 \times 10^{-9}\text{m}}{3.08\text{m}} = 1.85 \times 10^{-7}\text{rad} \tag{18}$$

Once we know the value of the angular diameter, the calculation of Betelgeuse's diameter is straightforward from Eq. (17)

$$b = a\theta = 1.6 \times 10^{18}\text{m} \times 1.85 \times 10^{-7}\text{rad} = 2.96 \times 10^{11}\text{m} \tag{19}$$

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# 8. Graphene nanoribbons

## Introduction

Graphene lacks an electronic band gap, limiting its application in electronic devices. However, graphene nanoribbons (Figure 2 (left)) exhibits different behavior. Let's estimate the band gap opening in graphene nanoribbons using an approximate energy dispersion evaluation as a function of the wave vector $k$. A suitable method to calculate the energy bands is the tight-binding approximation (TBA), which approximates the electronic wave function as a linear combination of atomic orbitals. The lattice periodicity is introduced via Bloch's theorem $\psi_k(x+na) = e^{ikna}\,\psi_k(x)$ where $a$ is the translation vector in 1D, and $n$ is an integer. In this exercise, we will restrict to interactions between nearest neighbors. As an example of TBA in a one-dimensional chain, consider an infinite polyacetylene carbon chain with single and double bonds (Figure 1(left)).

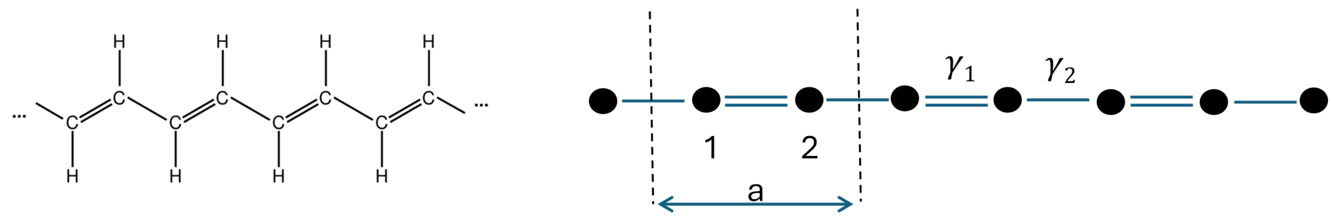



Figure 1: (left) Polyacetylene chain; (right) schematic representation

The unit cell in this case is composed of two atoms, labeled atom 1 and atom 2 (fig. 1 (right)). Within TBA the wavefunction can be expressed as a linear combination of the wavefunctions in the unit cell, $\psi^i(x)$, which can be written in terms of the atomic orbital wavefunctions $\phi_i(x)$, each weighted by a phase factor (Bloch's theorem):

$$\psi_k(x) = \zeta_1 \psi_k^1(x) + \zeta_2 \psi_k^2(x) \quad \text{with} \quad \psi_k^{1,2}(x) = \frac{1}{\sqrt{N_c}} \sum_{n=1}^{N_c} e^{ik(x+na)}\,\phi_{1,2}(x+na) \tag{1}$$

where $n$ runs over the $N_c$ unit cells. To solve the Schrödinger equation, we project it onto $\langle \psi_k^1|$ and $\langle \psi_k^2|$, resulting in a system of two equations. We assume that only nearest neighbor interactions are non-zero. The hopping integral $\langle \phi_i|H|\phi_j\rangle$ for the interaction between $1 \to 2$ is $\gamma_1$ and for the interaction between $2 \to 1$ is $\gamma_2$ (fig. 1b). The on-site energy, $\langle \phi_i|H|\phi_i\rangle = \varepsilon_0$ and the orbital overlap term $\langle \phi_i|\phi_j\rangle = \delta_{ij}$. This yields the eigenvalue equation (Eq. 2) that needs to be solved for the energy, $\varepsilon_k$. In summary, each term of the matrix accounts for interactions between $i$ and $j$, as shown by the rows and column labels, weighted by phase factors such as $e^{\pm ika}$, when interacting with nearest neighbors in different cells:

$$\begin{array}{c} \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cc} \quad 1 \quad\quad & \quad\quad 2 \quad \end{array} \\ \begin{bmatrix} \varepsilon_0 & \gamma_1 + \gamma_2\, e^{-ika} \\ \gamma_1 + \gamma_2\, e^{+ika} & \varepsilon_0 \end{bmatrix} \end{array} \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} = \varepsilon_k \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} \tag{2}$$

## Questions

Armchair graphene nanoribbons are one-dimensional, infinitely long linear chains with a width W, as illustrated in Figure 2 (left).

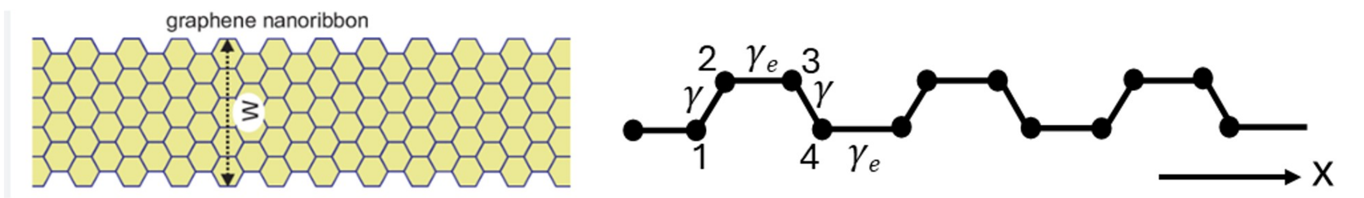


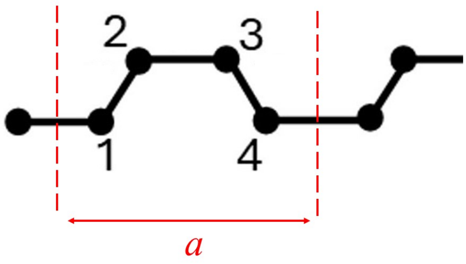

Figure:2 (left) armchair graphene nanoribbon; (right) schematic representation used for the TBA in this exercise

Our goal is to use tight-binding approximation, as explained in the introduction, to calculate the energy dispersion relation. As a simplification take the simplest infinite nanoribbon along direction $x$, as shown in fig. 2 (right). Assume the on-site energy, $\varepsilon_0$, is zero, and the hopping integral between nearest neighbors are $\gamma$ and $\gamma_e$ (fig. 2 (right)), with values $\gamma = -2.70$ eV and $\gamma_e = -3.02$ eV.

1. [**1 point**] Construct the unit cell.
2. [**1 point**] Write the wave function of an electronic orbital in the unit cell.
3. [**2.5 points**] Build the matrix of the eigenvalue equation, either by applying TBA or by similarity with Eq. (2).
4. [**2 points**] Calculate the energy gap at the $\Gamma$ point ($k = 0$).
5. [**1 point**] What would happen with the energy gap if the interaction between atoms in the nanoribbon is the same for all atoms, i.e. $\gamma = \gamma_e = -2.70$ eV?
6. [**2.5 points**] Make a schematic representation of: i) energy $E$ versus wave vector $k$ between 0 and $\pi/a$ for all the bands; ii) $E$ versus the density of states (DOS) for the valence band. Note: Recall that the DOS in 3D can be evaluated according to $g(E) = \frac{2}{(2\pi)^3} \int_S \frac{dS}{|\nabla_k E|}$, where the integral is performed on a constant energy surface, and the factor 2 accounts for spin degeneration.

## Solution

**1.)** (1 point) The unit cell is




**2.)** (1 point) Wave function of an electronic orbital in the unit cell.

In TBA we write the wave function as function of atomic wave functions. Since we have 4 atoms in the unit cell:

$$\psi_k(x) = \zeta_1 \psi_k^1(x) + \zeta_2 \psi_k^2(x) + \zeta_3 \psi_k^3(x) + \zeta_4 \psi_k^4(x)$$

where $j = 1, 2, 3, 4$ refers to the 4 atoms of the unit cell, with

$$\psi_k^j(x) = \frac{1}{\sqrt{N_c}} \sum_{n=1}^{N_c} e^{ik(x+na)}\, \phi_j(x + na)$$

**3.)** (2.5 points) Build the Hamiltonian matrix.

a) Easy (direct) way by comparing the case of polyacetylene chain, Eq. (2).

We take $\varepsilon_0 = 0$ and first neighbor interactions as $\gamma$ and $\gamma_e$; $\gamma$ for interactions $1 \leftrightarrow 2$ and $3 \leftrightarrow 4$, and $\gamma_e$ for interactions $2 \leftrightarrow 3$ and $1 \leftrightarrow 4$. We also apply phase factors between unit cells ($e^{\pm ika}$) when needed. One gets

$$\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{bmatrix} 0 & \gamma & 0 & \gamma_e e^{-ika} \\ \gamma & 0 & \gamma_e & 0 \\ 0 & \gamma_e & 0 & \gamma \\ \gamma_e e^{ika} & 0 & \gamma & 0 \end{bmatrix}$$

b) Standard procedure.

We need to solve the Schrödinger equation

$$\hat{H}|\psi\rangle = \varepsilon|\psi\rangle.$$

Therefore we project it over the 4 states $\langle\psi_k^i|$ to construct the Hamiltonian matrix:

$$\begin{bmatrix} H_{11} & H_{12} & H_{13} & H_{14} \\ H_{21} & H_{22} & H_{23} & H_{24} \\ H_{31} & H_{32} & H_{33} & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \end{bmatrix} = \varepsilon_k \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \end{bmatrix} \tag{3}$$

As an example, we calculate the first row by projecting over state $\langle\psi_k^1|$:

$$\begin{aligned} \langle\psi_k^1|H|\psi_k\rangle &= \langle\psi_k^1|H|\zeta_1\psi_k^1(x) + \zeta_2\psi_k^2(x) + \zeta_3\psi_k^3(x) + \zeta_4\psi_k^4(x)\rangle = \\ &= \zeta_1\langle\psi_k^1|H|\psi_k^1\rangle + \zeta_2\langle\psi_k^1|H|\psi_k^2\rangle + \zeta_3\langle\psi_k^1|H|\psi_k^3\rangle + \zeta_4\langle\psi_k^1|H|\psi_k^4\rangle. \end{aligned}$$

Now let us calculate one by one:

$$\begin{aligned} H_{11} = \langle\psi_k^1|H|\psi_k^1\rangle &= \frac{1}{N_c} \sum_{m,n}^{N_c} e^{ik(m-n)a}\, \langle\phi_1(x+na)|H|\phi_1(x+ma)\rangle \\ &= \langle\phi_1|H|\phi_1\rangle = \varepsilon_{0,1}\langle\phi_1|\phi_1\rangle = \varepsilon_{0,1} = \varepsilon_0 \end{aligned}$$

since $m = n$. Identically for $H_{22} = H_{33} = H_{44} \to \varepsilon_{0,2} = \varepsilon_{0,3} = \varepsilon_{0,4} = \varepsilon_0$. In addition, we considered $\varepsilon_0 = 0$.

Let us look at the interaction $1 \to 2$:

$$H_{12} = \langle \psi_k^1 | H | \psi_k^2 \rangle = \frac{1}{N_c} \sum_{m,n}^{N_c} e^{ik(m-n)a} \langle \phi_1(x+na) | H | \phi_2(x+ma) \rangle =$$
$$= \langle \phi_1 | H | \phi_2 \rangle = \gamma$$

since we only account for $1 \to 2$ in the same cell, i.e. $m = n$.

Since 1 and 3 are not nearest neighbors therefore $H_{13} = 0$.

Finally,

$$H_{14} = \langle \psi_k^1 | H | \psi_k^4 \rangle = \frac{1}{N_c} \sum_{m,n}^{N_c} e^{ik(m-n)a} \langle \phi_1(x+na) | H | \phi_4(x+ma) \rangle.$$

Now 1 is in cell $n$ and the interactions with 4 in cell $n-1$. Then

$$H_{14} = \frac{1}{N_c} \sum_{n}^{N_c} e^{ik(n-1-n)a} \langle \phi_1(x+na) | H | \phi_4(x+(n-1)a) \rangle =$$
$$= e^{-ika} \langle \phi_1 | H | \phi_4 \rangle = \gamma_e e^{-ika}.$$

Then the first row is

$$\begin{array}{ccccc} & 1 & 2 & 3 & 4 \\ 1 \to & 0 & \gamma & 0 & \gamma_e e^{-ika} \end{array}$$

By analogy we can proceed fast to write the elements of the matrix for $j = 2, 3, 4$:

$$\begin{bmatrix} 0 & \gamma & 0 & \gamma_e e^{-ika} \\ \gamma & 0 & \gamma_e & 0 \\ 0 & \gamma_e & 0 & \gamma \\ \gamma_e e^{ika} & 0 & \gamma & 0 \end{bmatrix}$$

**4.)** (2 points) In order to calculate the energy gap at the $\Gamma$ point ($k = 0$) we need to solve the Schrödinger equation in matrix form

$$\begin{bmatrix} 0 & \gamma & 0 & \gamma_e e^{-ika} \\ \gamma & 0 & \gamma_e & 0 \\ 0 & \gamma_e & 0 & \gamma \\ \gamma_e e^{ika} & 0 & \gamma & 0 \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \end{bmatrix} = \varepsilon_k \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \end{bmatrix} \tag{4}$$

which means $\det(\hat{H} - \varepsilon_k \cdot I) = 0$, i.e.

$$\begin{vmatrix} -\varepsilon_k & \gamma & 0 & \gamma_e e^{-ika} \\ \gamma & -\varepsilon_k & \gamma_e & 0 \\ 0 & \gamma_e & -\varepsilon_k & \gamma \\ \gamma_e e^{ika} & 0 & \gamma & -\varepsilon_k \end{vmatrix} =$$

$$= -\varepsilon_k \begin{vmatrix} -\varepsilon_k & \gamma_e & 0 \\ \gamma_e & -\varepsilon_k & \gamma \\ 0 & \gamma & -\varepsilon_k \end{vmatrix} - \gamma \begin{vmatrix} \gamma & 0 & \gamma_e e^{-ika} \\ \gamma_e & -\varepsilon_k & \gamma \\ 0 & \gamma & -\varepsilon_k \end{vmatrix} - \gamma_e \begin{vmatrix} \gamma & 0 & \gamma_e e^{-ika} \\ -\varepsilon_k & \gamma_e & 0 \\ \gamma_e & -\varepsilon_k & \gamma \end{vmatrix} = ... = \varepsilon_k^4 - S_1 \varepsilon_k^2 + S_2 = 0,$$

with

$$S_1 = 2(\gamma^2 + \gamma_e^2), \qquad S_2 = \gamma^4 + \gamma_e^4 - 2\gamma^2\gamma_e^2 \cos ka.$$

Then,

$$\varepsilon_k^2 = \frac{1}{2}\left( S_1 \pm \sqrt{S_1^2 - 4S_2} \right)$$

and one obtains 4 solutions, i.e. 4 bands, with energies:

$$\begin{aligned}
1 \rightarrow &\quad +\sqrt{\gamma^2+\gamma_e^2+\sqrt{2}\,\gamma\gamma_e\sqrt{1+\cos ka}} \\
2 \rightarrow &\quad +\sqrt{\gamma^2+\gamma_e^2-\sqrt{2}\,\gamma\gamma_e\sqrt{1+\cos ka}} \\
3 \rightarrow &\quad -\sqrt{\gamma^2+\gamma_e^2+\sqrt{2}\,\gamma\gamma_e\sqrt{1+\cos ka}} \\
4 \rightarrow &\quad -\sqrt{\gamma^2+\gamma_e^2-\sqrt{2}\,\gamma\gamma_e\sqrt{1+\cos ka}}
\end{aligned}$$

At the point $\Gamma(k=0)$, introducing the values for $\gamma$ and $\gamma_e$, one finds

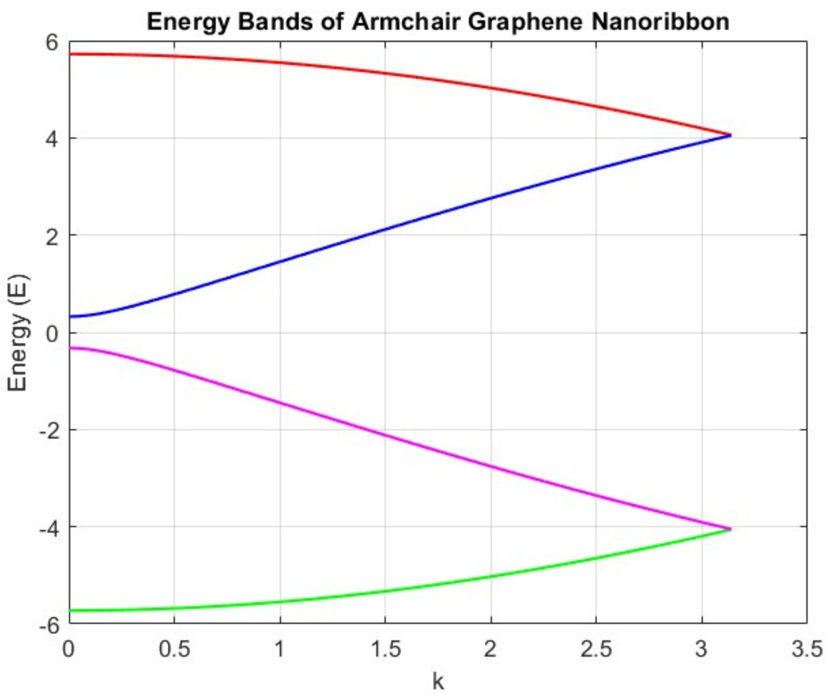
$$\begin{aligned}
1 \rightarrow &\quad +5.724\,\mathrm{eV} \\
2 \rightarrow &\quad +0.324\,\mathrm{eV} \\
3 \rightarrow &\quad -5.724 \\
4 \rightarrow &\quad -0.324\,\mathrm{eV}
\end{aligned}$$

Then, the opening of the band gap at $\Gamma$ is the difference between 2 and 4:

$$E_{gap} = 0.648\,\mathrm{eV}.$$

**5.)** (1 point) If the interaction between atoms in the nanoribbon is the same for all atoms $\gamma = \gamma_e = -2.70$ eV, the opening of the gap is zero, $E_{gap} = 0$. This is the situation for graphene!

**6.)** i) The graph of the energy versus $k$ obtained from the above expressions has the form displayed in fig. 3 (0.75 points).




ii) $E$ versus DOS (1.75 points)

Finally, let us see that the density of states diverges for a 1D structure at the $\Gamma$ point ($k=0$). In 3D the DOS is

$$g(E) = \frac{2}{(2\pi)^3}\int_S \frac{dk_x dk_y}{|\nabla_k E|},$$

where the integral extends to the surface of constant energy. In 1D the integral can only take 2 values of constant energy, then

$$g(E) = \frac{2}{2\pi}\frac{2}{|dE/dk|}.$$

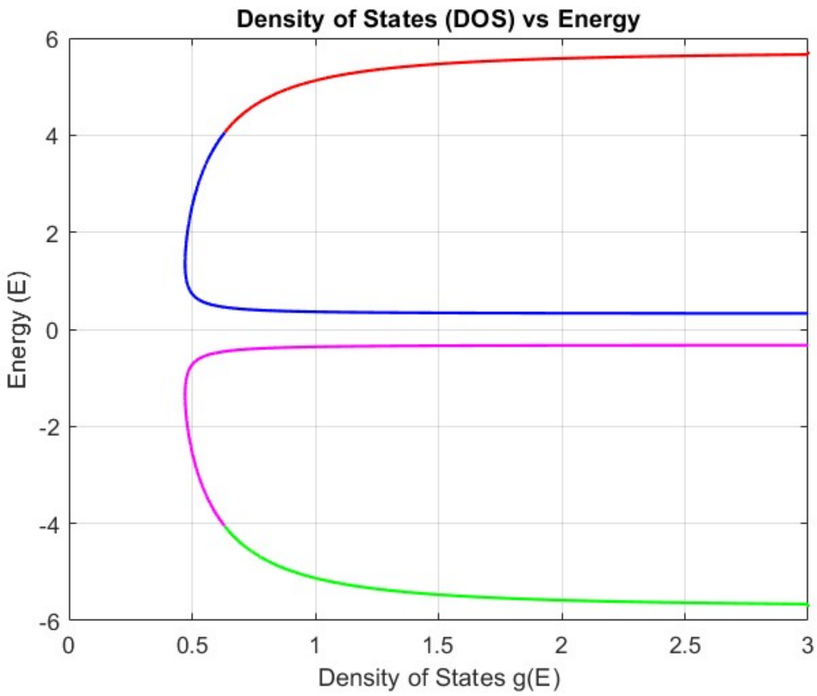
We found

$$\varepsilon_k = \pm\sqrt{\gamma^2 + \gamma_e^2 \pm \sqrt{2}\,\gamma\gamma_e\sqrt{1+\cos ka}} \equiv \pm\Big(A \pm B\,(1+\cos ka)^{1/2}\Big)^{1/2}$$

so that

$$\begin{aligned} g(\varepsilon) &= \frac{8}{\pi a}\frac{\Big(A \pm B\,(1+\cos ka)^{1/2}\Big)^{1/2}(1+\cos ka)^{1/2}}{\sin ka} = \\ &= \frac{8}{\pi a B}\frac{\varepsilon_k\left(\frac{\varepsilon_k^2 - A}{B}\right)}{\sin ka} \end{aligned}$$

Clearly, this expression diverges at $k \to 0$ (since $\sin ka \to 0$), which is the typical behaviour for 1D structures. The plot is as follows (only the schematic representation of the valence band is requested):

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# 9. Quantum Grover algorithm and classical collisions

The **quantum Grover algorithm** is an oracle algorithm that can find a register in an unstructured list of $N$ registers (Imagine finding a name in a telephone book if we are given the telephone number).
The idea is to start with an equally weighted state of all registers:

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle,$$

and do some operations that enhance the amplitude of the marked register denoted by $|w\rangle$. One first writes $|\psi_0\rangle$ in a two-dimensional basis

$$|\psi_0\rangle = \sqrt{\frac{N-1}{N}}|\alpha\rangle + \sqrt{\frac{1}{N}}|w\rangle,$$

where $|\alpha\rangle$ is the state of all unmarked registers (of course, $\langle\alpha|w\rangle = 0$). In the $\{|\alpha\rangle, |w\rangle\}$ basis, the oracle is given by a unitary matrix

$$U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

that adds a phase, $-1$, to the amplitude of the marked state $|w\rangle$. The Grover algorithm is the following:

(I) Apply the oracle $U$

(II) Do a unitary operation that can be seen as a reflection over $|\psi_0\rangle$

$$K = 2|\psi_0\rangle\langle\psi_0| - \mathbb{1},$$

(III) Repeat operations (I) and (II) until the amplitude of $|w\rangle$ is maximal, i.e. when measuring the state after these iterations one obtains $|w\rangle$ with maximum probability.

1. [**2 points**] Show that $KU$ can be written as a rotation matrix $G(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, and find the $\theta$ as a function of $N$.
2. [**2 points**] Show that if $N = 4$, one iteration of the Grover algorithm is sufficient to find the marked state. [Recall that $\cos\theta/2 = \sqrt{(1+\cos\theta)/2}$ and $\sin\theta/2 = \sqrt{(1-\cos\theta)/2}$].
3. [**2 points**] Find the general expression of $N$ (although in general, it will not be a natural number) in terms of the number of times, $n$, the oracle must be called for the Grover algorithm to find the exact marked state. For solutions of large $N$, use the Taylor expansion to find the asymptotic expression of $n$ as a function of $N$.

It is interesting to realize that the quantum Grover algorithm is formally equivalent to the following **classical scattering problem**. Imagine a dystopian classical world where energy has become very scarce. In this scenario, we aim to design a mountain train that operates without consuming energy, relying solely on the physics of elastic collisions.

The train consists of two parts: a locomotive without an engine of mass $m_1$ and a coach of mass $m_2$, with $m_1 > m_2$. The locomotive is positioned at the rear, while the coach leads at the front. Starting from rest at an initial height on a mountain, the train descends toward a bottom station, reaching a final velocity $v = 1$ (in arbitrary units).

Although the train's components descend simultaneously, they are not physically connected. Upon reaching the bottom station, the coach collides with a wall, reversing its velocity, and subsequently collides with the locomotive. These collisions may be repeated multiple times. All collisions are assumed to be perfectly elastic and to occur sequentially.

4. [**2 points**] Demonstrate that this classical scattering problem is formally equivalent to the operations of the Grover algorithm, where the oracle $U$ corresponds to the collision of $m_2$ with the bottom wall and $K$ represents the locomotive-coach collisions. Derive the expressions relating $m_1$ and $m_2$ to $N$.

   *Hint*: The following rescaling of the velocities is very useful: $\xi_i = \sqrt{m_i/M}\, v_i$ where $M = m_1 + m_2$. To ease the notation, it is also convenient to define the ratio $\eta = m_1/m_2$.

5. [**2 points**] What is the minimum mass ratio, $\eta = m_1/m_2$ (with $\eta > 1$), required for the coach to remain stopped at the bottom station after the train descends?

6. [**1 point**] If the train took a time $T$ to descend, how much time do passengers have to do their shopping before the locomotive returns to the bottom station after reaching its maximum height? (assume the mountain is a sloped plane)

7. [**2 points**] In the above scenario, when the locomotive reaches the bottom station it collides with the stopped coach and a second round of collisions occurs. When this round ends, what are the final velocities of the coach and the locomotive?

8. [**2 points**] Derive the general expression for the mass ratio $\eta$ under which this "park-and-pick-up" phenomenon occurs.

## Solution

**1.)** *(2 points)* Show that $KU$ can be written as a rotation matrix $G(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, and find the $\theta$ as a function of $N$.

$$K = 2|\psi_0\rangle\langle\psi_0| - \mathbb{1} = \begin{pmatrix} (N-2)/N & 2\sqrt{N-1}/N \\ 2\sqrt{N-1}/N & (2-N)/N \end{pmatrix},$$

$$KU = \begin{pmatrix} (N-2)/N & 2\sqrt{N-1}/N \\ 2\sqrt{N-1}/N & (2-N)/N \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} (N-2)/N & -2\sqrt{N-1}/N \\ 2\sqrt{N-1}/N & (N-2)/N \end{pmatrix},$$

Defining $\cos\theta = \frac{N-2}{N}$ and $\sin\theta = 2\frac{\sqrt{N-1}}{N} \to KU = G(\theta)$.

**2.)** *(2 points)* Show that if $N = 4$, one iteration of the Grover algorithm is sufficient to find the marked state. [Recall that $\cos\theta/2 = \sqrt{(1+\cos\theta)/2}$ and $\sin\theta/2 = \sqrt{(1-\cos\theta)/2}$].

Note that $\cos\theta/2 = \sqrt{\dfrac{1+\cos\theta}{2}} = \sqrt{\dfrac{N-1}{N}}$ and $\sin\theta/2 = \sqrt{\dfrac{1-\cos\theta}{2}} = \sqrt{\dfrac{1}{N}}$. Thus,

$$|\psi_0\rangle = \begin{pmatrix} \sqrt{\frac{N-1}{N}} \\ \sqrt{\frac{1}{N}} \end{pmatrix} = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix}.$$

Then,

$$KU|\psi_0\rangle = |w\rangle \Rightarrow G(\theta)\begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix} = \begin{pmatrix} \cos(\theta+\theta/2) \\ \sin(\theta+\theta/2) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

$$\theta + \theta/2 = \pi/2 \Rightarrow \theta = \frac{\pi}{3},$$

$$\sin^2\theta/2 = \frac{1}{N} \to N = \frac{1}{\sin^2\frac{\pi}{6}} = 4.$$

One can also find this result directly by substituting $N = 4$ in the expressions of $KU$ and $|\psi_0\rangle$:

$$KU|\psi_0\rangle = \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ \sqrt{3/2} & 1/2 \end{pmatrix} \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

**3.)** *(2 points)* Find the general expression of $N$ (although in general, it will not be a natural number) in terms of the number of times, $n$, the oracle must be called for the Grover algorithm to find the exact marked state. For solutions of large $N$, use the Taylor expansion to find the asymptotic expression of $n$ as a function of $N$.

$$[G(\theta)]^n|\psi_0\rangle = G(n\theta)|\psi_0\rangle|w\rangle \Rightarrow \begin{pmatrix} \cos n\theta & -\sin n\theta \\ \sin n\theta & \sin n\theta \end{pmatrix} \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \end{pmatrix} = \begin{pmatrix} \cos(n\theta+\theta/2) \\ \sin(n\theta+\theta/2) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$n\theta + \theta/2 = \pi/2 \Rightarrow \theta = \frac{\pi}{2n+1}$$

$$\sin^2\theta/2 = \frac{1}{N} \to N = \left[\sin^2\frac{\pi}{2(2n+1)}\right]^{-1}$$

$$N - 1 = \cot^2\frac{\pi}{2(2n+1)}.$$

Note that $n = 1$ gives $N = 4$.
For large $N$

$$N \simeq \frac{4(2n+1)^2}{\pi^2} \simeq \frac{16}{\pi^2}n^2 \Rightarrow n \simeq \frac{\pi}{4}\sqrt{N}.$$

**4.)** *(2 points)* Demonstrate that this classical scattering problem is formally equivalent to the operations of the Grover algorithm, where the oracle $U$ corresponds to the collision of $m_2$ with the bottom wall and $K$ represents the locomotive-coach collisions. Derive the expressions relating $m_1$ and $m_2$ to $N$.

*Hint*: The following rescaling of the velocities is very useful: $\xi_i = \sqrt{m_i/M}\, v_i$ where $M = m_1 + m_2$. To ease the notation, it is also convenient to define the ratio $\eta = m_1/m_2$.

We take the convention that the positive direction is downwards and impose energy and momentum conservation.

The rescaling $\xi_i = \sqrt{m_i/M} v_i$ renders the energy conservation equation equivalent to the conservation of the modulus of the vector $\vec{\xi}$

$$\xi_1^2 + \xi_2^2 = \xi_1'^2 + \xi_2'^2 = 1$$

Momentum conservation reads

$$\sqrt{m_1}\xi_1 + \sqrt{m_2}\xi_2 = \sqrt{m_1}\xi_1' + \sqrt{m_2}\xi_2'$$

On can easily solve these equations to get

$$\begin{pmatrix}\xi_1'\\ \xi_2'\end{pmatrix} = \begin{pmatrix}(m_1-m_2)/(m_1+m_2) & 2\sqrt{m_1m_2}/(m_1+m_2)\\ 2\sqrt{m_1m_2}/(m_1+m_2) & (m_2-m_1)/(m_1+m_2)\end{pmatrix}\begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix} = S\begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix}.$$

Defining $\eta = m_1/m_2$, the matrix $S$ can be rewritten as

$$S = \begin{pmatrix}(\eta-1)/(\eta+1) & 2\sqrt{\eta}/(\eta+1)\\ 2\sqrt{\eta}/(\eta+1) & -(\eta-1)/(\eta+1)\end{pmatrix}.$$

The collision with the wall can be introduced as

$$U = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

such that

$$SU = \begin{pmatrix}(\eta-1)/(\eta+1) & -2\sqrt{\eta}/(\eta+1)\\ 2\sqrt{\eta}/(\eta+1) & (\eta-1)/(\eta+1)\end{pmatrix}$$

is a rotation of angle $\theta$, $SU = G(\theta)$ (defined in 1) with

$$\cos\theta = \frac{\eta-1}{\eta+1},\ \ \sin\theta = 2\frac{\sqrt{\eta}}{\eta+1},\ \text{ and }\ \eta = \cot^2\theta/2.$$

**5.)** *(2 points)* What is the minimum mass ratio, $\eta = m_1/m_2$ (with $\eta > 1$), required for the coach to remain stopped at the bottom station after the train descends?

The initial state, considering $v_1 = v_2 = v = 1$ can be written as

$$\vec{\xi} = \begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix} = \begin{pmatrix}\sqrt{\eta/(\eta+1)}\\ 1/\sqrt{\eta+1}\end{pmatrix} = \begin{pmatrix}\cos\theta/2\\ \sin\theta/2\end{pmatrix},$$

Then, if the coach remains stopped at the bottom station after the first collision ($v_2' = 0$) and the locomotive goes up to the mountain

$$SU\vec{\xi} = G(\theta)\begin{pmatrix}\cos\theta/2\\ \sin\theta/2\end{pmatrix} = \begin{pmatrix}\cos(\theta+\theta/2)\\ \sin(\theta+\theta/2)\end{pmatrix} = \begin{pmatrix}-1\\ 0\end{pmatrix}.$$

and thus, $\frac{3\theta}{2} = \pi \to \theta = \frac{2\pi}{3}$. The mass ratio is $\eta = \frac{m_1}{m_2} = \cot^2\frac{\pi}{3} = \frac{1}{3}$, which means that the coach can not remain stopped at the bottom station after the first collision unless $m_1 < m_2$. Then, we need to consider a second collision

$$G^2(\theta)\vec{\xi} = \begin{pmatrix}\cos 2\theta & -\sin 2\theta\\ \sin 2\theta & \sin 2\theta\end{pmatrix}\begin{pmatrix}\cos\theta/2\\ \sin\theta/2\end{pmatrix} = \begin{pmatrix}\cos(2\theta+\theta/2)\\ \sin(2\theta+\theta/2)\end{pmatrix} = \begin{pmatrix}-1\\ 0\end{pmatrix}.$$

In this case $\theta = \dfrac{2\pi}{5}$, $\eta = \cot^2\dfrac{\pi}{5} = 1 + \dfrac{2}{\sqrt{5}} > 1$ and $\vec{\xi} = \begin{pmatrix}\cos(\pi/5)\\ \sin(\pi/5)\end{pmatrix}$.

From the equation in terms of $\eta$: $(KU)^2\vec{\xi} = \begin{pmatrix}-1\\ 0\end{pmatrix}$ we arrive at $5\eta^2 - 10\eta + 1 = 0$ which directly gives $\eta = 1 + 2/\sqrt{5} = \cot^2(\pi/5)$ (which is a way of finding this trigonometric expression).

**6.)** *(1 point)* If the train took a time $T$ to descend, how much time do passengers have to do their shopping before the locomotive returns to the bottom station after reaching its maximum height? (assume the mountain is a sloped plane)

If $v_2' = 0$, energy conservation implies that $v_1' = \sqrt{\frac{m_1 + m_2}{m_1}} = \sqrt{\frac{1+\eta}{\eta}}$.

Since $T \propto v$:

$$T' = 2\frac{v_1'}{v_1}T = 2\sqrt{\frac{1+\eta}{\eta}}T = 2(\sqrt{5}-1)T = 2.47\,T.$$

Recall that $v_1 = v_2 = v = 1$.

**7.)** *(2 points)* In the above scenario, when the locomotive reaches the bottom station it collides with the stopped coach and a second round of collisions occurs. When this round ends, what are the final velocities of the coach and the locomotive?

Before the second round of collisions, the rescaled velocity vector is $\xi^{(2)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Notice that now there is a first locomotive-coach collision and then a reflection, i.e. we have the sequence $US$. Observe that $US = (SU)^{-1})$, i.e. $US = G(-\theta)$.

$$US\xi^{(2)} = G(-2\pi/5)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(2\pi/5) \\ -\sin(2\pi/5) \end{pmatrix}.$$

Since $\cos(2\pi/5)$ and $\sin(2\pi/5) > 0$, there is a second sequence of collisions

$$(US)(US)\xi^{(2)} = G(-4\pi/5)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(4\pi/5) \\ -\sin(4\pi/5) \end{pmatrix} = -\begin{pmatrix} \cos(\pi/5) \\ \sin(\pi/5) \end{pmatrix}.$$

The velocities are identical to the initial ones (see 5), but reversed.

**8.)** *(2 points)* Derive the general expression for the mass ratio $\eta$ under which this "park-and-pick-up" phenomenon occurs.

$$G^n(\theta)\xi = G(n\theta)\xi = \begin{pmatrix} \cos(n+1/2)\theta \\ \sin(n+1/2)\theta \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \Rightarrow \theta_n = \frac{2\pi}{2n+1} \Rightarrow \eta_n = \cot^2\frac{\pi}{2n+1},$$

where $n$ is the number of locomotive-coach collisions until the coach remains stopped. As shown in 5, the $n = 1$ value ($\eta_1 = 1/3$) is also a valid mass ratio, but corresponds to a case where $m_1 < m_2$.

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