

1 Classical Mechanics

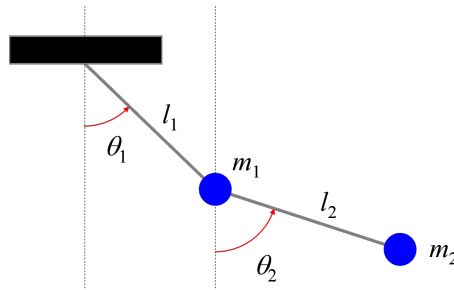


Figure 1: Sketch of the double pendulum system.

The double pendulum is a system consisting of two simple pendulums, one of which is attached to the other, as it is shown in Fig. 1. Motion is contained within a vertical plane, so there are only two degrees of freedom, namely, the angles θ_1 and θ_2 made by each wire with the vertical direction.

Let us assume that both wires have the same length, i.e., $l_1 = l_2 = \ell$, and their respective masses can be neglected. Moreover, we also assume the same mass for both pendulums, that is, $m_1 = m_2 = m$.

Whether the double pendulum displays either a regular or a chaotic behavior depends on the initial conditions.

1. **(6 points)** Determine the equations of motion of the two pendulums from their Lagrangian.
2. **(2 points)** Suggest two initial conditions that correspond to two unstable trajectories. Calculate their mechanical energy.
3. **(2 points)** Could you suggest any initial condition leading to regular motion?

Solutions

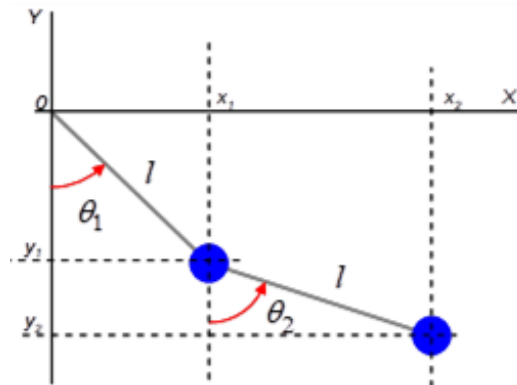


Figure 2: Sketch of the double pendulum system specifying the angular variables of interest to describe the system dynamics.

To simplify the calculations, we first define the following variables according to Fig. 2:

$$\begin{aligned}x_1 &= l \sin \theta_1, \\y_1 &= -l \cos \theta_1, \\x_2 &= l \sin \theta_1 + l \sin \theta_2 = l (\sin \theta_1 + \sin \theta_2), \\y_2 &= -l \cos \theta_1 - l \cos \theta_2 = -l (\cos \theta_1 + \cos \theta_2).\end{aligned}$$

- (6 points)** Determine the equations of motion of the two pendulums from their Lagrangian.

The potential energy is $V = V_1 + V_2$. If we take $y = 0$ as the zero for the potential energy, then

$$\begin{aligned}V_1 &= mgy_1 = -mgl \cos \theta_1, \\V_2 &= mgy_2 = -mgl (\cos \theta_1 + \cos \theta_2).\end{aligned}$$

On the other hand, the kinetic energy is $T = T_1 + T_2$, where

$$\begin{aligned}T_1 &= \frac{1}{2}mv_1^2 = \frac{1}{2}m(\dot{x}_1^2 + \dot{y}_1^2) = \frac{1}{2}ml^2\dot{\theta}_1^2, \\T_2 &= \frac{1}{2}mv_2^2 = \frac{1}{2}m(\dot{x}_2^2 + \dot{y}_2^2) = \frac{1}{2}ml^2 \left[\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1\dot{\theta}_2 \cos(\theta_1 - \theta_2) \right].\end{aligned}$$

From them, we obtain the Lagrangian for the system,

$$\mathcal{L} = T - V = \frac{1}{2}ml^2 \left[2\dot{\theta}_1^2 + \dot{\theta}_2^2 + 2\dot{\theta}_1\dot{\theta}_2 \cos(\theta_1 - \theta_2) \right] + mgl (2 \cos \theta_1 + \cos \theta_2).$$

The Lagrangian equations for each pendulum read as

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_i} \right) - \frac{\partial \mathcal{L}}{\partial \theta_i} = 0,$$

with $i = 1, 2$. Making the corresponding substitutions, we finally obtain the equations of motion for the double pendulum, which read as:

$$\begin{aligned}2m\ell^2\ddot{\theta}_1 + m\ell^2\ddot{\theta}_2 \cos(\theta_1 - \theta_2) + m\ell^2\dot{\theta}_2^2 \sin(\theta_1 - \theta_2) + 2mgl \sin \theta_1 &= 0, \\m\ell^2\ddot{\theta}_2 + m\ell^2\ddot{\theta}_1 \cos(\theta_1 - \theta_2) - m\ell^2\dot{\theta}_1^2 \sin(\theta_1 - \theta_2) + mgl \sin \theta_2 &= 0,\end{aligned}$$

or, after removing constant factors, as:

$$\begin{aligned}2\ddot{\theta}_1 + \ddot{\theta}_2 \cos(\theta_1 - \theta_2) + \dot{\theta}_2^2 \sin(\theta_1 - \theta_2) + 2\omega^2 \sin \theta_1 &= 0, \\\ddot{\theta}_2 + \ddot{\theta}_1 \cos(\theta_1 - \theta_2) - \dot{\theta}_1^2 \sin(\theta_1 - \theta_2) + \omega^2 \sin \theta_2 &= 0,\end{aligned}$$

where $\omega \equiv \sqrt{g/\ell}$ corresponds to the oscillation frequency for a simple pendulum.

2. (2 points) Suggest two initial conditions that correspond to two unstable trajectories. Calculate their mechanical energy.

The following initial conditions, $(\theta_1(0), \theta_2(0), \dot{\theta}_1(0), \dot{\theta}_2(0))$, are unstable:

- Initial condition 1: $(0, \pi, 0, 0)$, with $E_1 = -mgl$.
- Initial condition 2: $(\pi, \pi, 0, 0)$, with $E_2 = 3mgl$.

3. (2.5 points) Could you suggest any initial condition leading to regular motion?

At high energies, $T \gg V$ and $\theta_1 \approx \theta_2$. Accordingly, $\mathcal{L} \approx T$ and the equations of motion are

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\theta}_i} \right) = 0,$$

that is, $\ddot{\theta}_i = 0$, where $i = 1, 2$. The solution to this equation of motion is $\theta_i(t) = c_i t$, which is the trajectory for a rotor.

2 Classical Gravitation

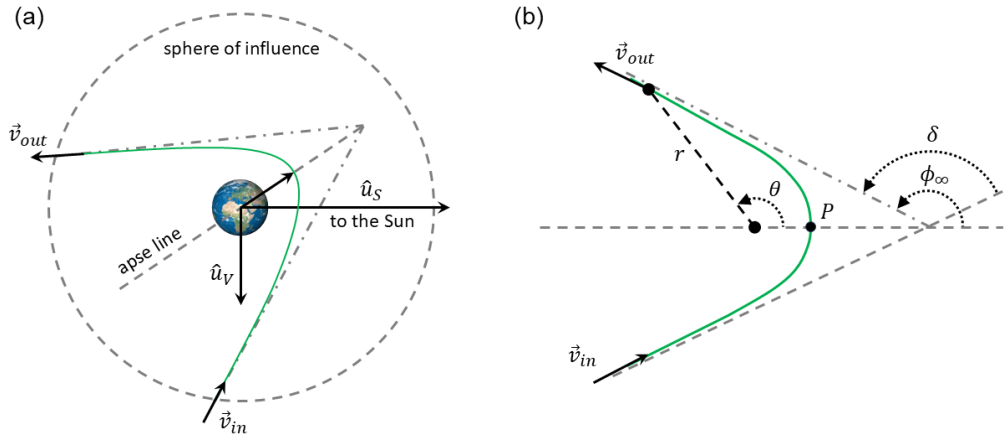


Figure 3: (a) Hyperbolic flyby trajectory within the sphere of influence in the frame oriented by the Sun direction. (b) Hyperbolic trajectory in the frame oriented by the apse line showing polar coordinates and relevant angles.

A planet's gravitational sphere of influence is the region near the planet where its attraction overwhelms all other gravitational forces, including that of the Sun. Relative to the planet, the sphere of influence can be considered to be of infinite radius.

A spacecraft that enters a planet's sphere of influence and does not impact the planet or go into orbit around it will continue in its hyperbolic trajectory through periapsis P and exit the sphere of influence, as it is shown in Fig. 3(a).

Let \hat{u}_V be the unit vector in the direction of the planet's heliocentric velocity vector \vec{V} —that will be taken as constant neglecting its change of direction during the flyby—, and let \hat{u}_S be the unit vector pointing from the planet to the Sun. Consider a circular planetary orbit with \hat{u}_S and \hat{u}_V orthogonal. The initial heliocentric velocity of the spacecraft when it enters into the planet's sphere of influence is

$$\vec{V}_{in} = V_{in} (\cos \alpha \hat{u}_V + \sin \alpha \hat{u}_S),$$

where α is the angle between \vec{V}_{in} and \vec{V} (we use uppercase letters for the heliocentric velocities and lowercase for the geocentric ones). In the planet's reference frame, this velocity is

$$\vec{v}_{in} = v_\infty (\cos \phi_\infty \hat{u}_V + \sin \phi_\infty \hat{u}_S).$$

The spacecraft flies past the planet on the sunlit side [see Fig. 3(a)]. It follows a Keplerian trajectory that, in the planet's reference frame oriented by the apse line [see Fig. 3(b)], is given by

$$\frac{1}{r} = \frac{\mu}{h^2} (1 + e \cos \theta),$$

where $h = |\vec{L}|/m$ is the spacecraft angular momentum per unit mass, $\mu = GM_{\text{planet}}$, e is the eccentricity, and r and θ are the polar coordinates (radial distance and polar angle) in that frame.

- (1 point)** Write \vec{v}_{in} and ϕ_∞ in terms of V_{in} , α , and V .
- (5 points)** Determine the eccentricity e of the trajectory and the total angular deviation δ of the spacecraft as a function of the initial speed v_∞ and the periapsis radius r_P .
- (4 points)** Let the spacecraft's final heliocentric velocity be $\vec{V}_{out} = V_{out} (\cos \alpha_{out} \hat{u}_V + \sin \alpha_{out} \hat{u}_S)$. Determine V_{out} and α_{out} in terms of the initial velocities V , V_{in} , the orientation α , and the periapsis radius r_P .

Solutions

1. (1 point) Write \vec{v}_{in} and ϕ_{∞} in terms of V_{in} , α , and V .

The geocentric spacecraft velocity is $\vec{v}_{\text{in}} = \vec{V}_{\text{in}} - \vec{V}$, i.e.,

$$\vec{v}_{\text{in}} = (V_{\text{in}} \cos \alpha - V) \hat{u}_V + V_{\text{in}} \sin \alpha \hat{u}_S.$$

This can be written as in the text,

$$\vec{v}_{\text{in}} = v_{\infty} (\cos \phi_{\infty} \hat{u}_V + \sin \phi_{\infty} \hat{u}_S),$$

with

$$\begin{aligned} v_{\infty} &= \sqrt{V^2 + V_{\text{in}}^2 - 2VV_{\text{in}} \cos \alpha}, \\ \tan \phi_{\infty} &= \frac{V_{\text{in}} \sin \alpha}{V_{\text{in}} \cos \alpha - V}. \end{aligned}$$

2. (5 points) Determine the eccentricity e of the trajectory and the total angular deviation δ of the spacecraft as a function of the initial speed v_{∞} and the periapsis radius r_P .

Both, energy and angular momentum, are conserved in the inertial geocentric frame, so that

$$\begin{aligned} \frac{1}{2}v_{\infty}^2 &= \frac{1}{2}v_P^2 - \frac{\mu}{r_P}, \\ h &= r_P v_P. \end{aligned}$$

Also, r_P is the minimum radius ($\cos \theta = 1$), i.e.,

$$r_P = \frac{h^2}{\mu} \frac{1}{1+e},$$

so that the eccentricity is

$$e = 1 + \frac{r_P v_{\infty}^2}{\mu}.$$

On the other hand, $r \rightarrow \infty$ when the spacecraft crosses the planet sphere of influence with the polar angle becoming $\cos \theta_{\infty} = -1/e$. The deviation is $\delta = \pi - 2\beta$, with $\beta = \pi - \theta_{\infty}$. This leads to

$$\cos \beta = -\cos \theta_{\infty} = \frac{1}{e},$$

which leads to

$$\sin \frac{\delta}{2} = \sin \left(\frac{\pi}{2} - \beta \right) = \cos \beta = \frac{1}{e}.$$

Finally,

$$\delta = 2 \arcsin \left(\frac{1}{e} \right) = 2 \arcsin \left(\frac{1}{1 + \frac{r_P v_{\infty}^2}{\mu}} \right).$$

3. (4 points) Let the spacecraft's final heliocentric velocity be $\vec{V}_{\text{out}} = V_{\text{out}} (\cos \alpha_{\text{out}} \hat{u}_V + \sin \alpha_{\text{out}} \hat{u}_S)$. Determine V_{out} and α_{out} in terms of the initial velocities V , V_{in} , the orientation α , and the periapsis radius r_P .

Let

$$\vec{v}_{\text{out}} = v_{\text{out}} (\cos \phi_{\text{out}} \hat{u}_V + \sin \phi_{\text{out}} \hat{u}_S).$$

Due to energy conservation $v_{\text{out}} = v_{\infty}$. The spacecraft velocity also rotates at an angle δ with respect to the incoming velocity, so that $\phi_{\text{out}} = \phi_{\infty} + \delta$. Finally,

$$\vec{v}_{\text{out}} = v_{\infty} [\cos(\phi_{\infty} + \delta) \hat{u}_V + \sin(\phi_{\infty} + \delta) \hat{u}_S].$$

The final heliocentric velocity will be:

$$\vec{V}_{\text{out}} = \vec{v}_{\text{out}} + \vec{V} = [v_{\infty} \cos(\phi_{\infty} + \delta) + V] \hat{u}_V + v_{\infty} \sin(\phi_{\infty} + \delta) \hat{u}_S.$$

This can be written as

$$\vec{V}_{\text{out}} = V_{\text{out}} (\cos \alpha_{\text{out}} \hat{u}_V + \sin \alpha_{\text{out}} \hat{u}_S).$$

After some algebra,

$$\begin{aligned} V_{\text{out}} &= \sqrt{v_{\infty}^2 + V^2 + 2v_{\infty}V \cos(\phi_{\infty} + \delta)}, \\ \alpha_{\text{out}} &= \arctan \left[\frac{v_{\infty} \sin \phi_{\infty}}{v_{\infty} \cos(\phi_{\infty} + \delta) + V} \right], \end{aligned}$$

where v_{∞} , ϕ_{∞} , and δ are given by the data V , V_{in} , α , and r_P , as

$$\begin{aligned} v_{\infty} &= \sqrt{V^2 + V_{\text{in}}^2 - 2VV_{\text{in}} \cos \alpha}, \\ \phi_{\infty} &= \arctan \left(\frac{V_{\text{in}} \sin \alpha}{V_{\text{in}} \cos \alpha - V} \right), \\ \delta &= 2 \arcsin \left[\frac{1}{1 + \frac{r_P}{\mu} (V^2 + V_{\text{in}}^2 - 2VV_{\text{in}} \cos \alpha)} \right]. \end{aligned}$$

3 Electromagnetism

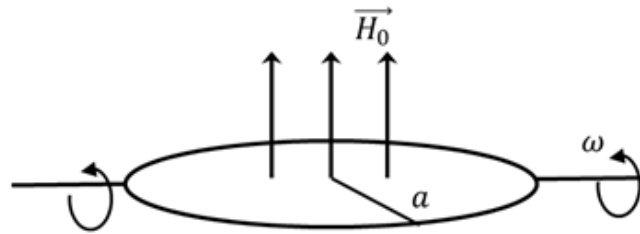


Figure 4: Sketch of the rotating ring and the direction of the external constant magnetic field.

A thin copper ring rotates in free space about an axis perpendicular to a uniform magnetic field \vec{H}_0 , as it is shown in Fig. 4. Its initial frequency of rotation is ω_0 .

Data: $\sigma_{\text{Cu}} = 58.7 \times 10^6 \text{ S/m}$, $\rho_{\text{Cu}} = 8.9 \text{ g}\cdot\text{cm}^{-3}$.

1. **(10 points)** Calculate the time it takes the frequency to decrease to $1/e$ of its original value under the assumption that the energy goes into Joule heat, for $H_0 = 15.9 \text{ kA}\cdot\text{m}^{-1}$ and a radius for the ring $a = 1 \text{ cm}$.

Solutions

1. (10 points) Calculate the time it takes the frequency to decrease to $1/e$ of its original value under the assumption that the energy goes into Joule heat, for $H_0 = 15.9 \text{ kA}\cdot\text{m}^{-1}$ and a radius for the ring $a = 1 \text{ cm}$.

The first thing to calculate is the voltage developed in the wire while rotating with angular frequency ω applying Faraday's law:

$$\mathcal{E} = -\frac{d\varphi_B}{dt} = \mu_0 H_0 \pi a^2 \omega \sin \omega t.$$

From \mathcal{E} it can be calculated the current in the ring I :

$$\mathcal{E} = IR,$$

where R is the electrical resistance:

$$I = \frac{\mu_0 H_0 \pi a^2 \omega \sin \omega t}{R}.$$

The average power loss to Joule heating per cycle is:

$$P = \langle I^2 \rangle R = \frac{(\mu_0 H_0 \pi a^2 \omega)^2}{2R}.$$

The source for this heating is the kinetic energy of the ring:

$$E_{\text{kin}} = \frac{I_{\text{in}} \omega^2}{2},$$

where I_{in} is the moment of inertia about the axis of rotation of the ring:

$$I_{\text{in}} = \frac{ma^2}{2},$$

with m the mass of the ring.

The power loss is due to the reduction in kinetic energy:

$$\frac{d}{dt} \left(\frac{ma^2 \omega^2}{4} \right) = -\frac{(\mu_0 H_0 \pi a^2 \omega)^2}{2R}.$$

The solution of this equation is:

$$\omega = \omega_0 e^{-t/\tau},$$

with

$$\tau = \frac{mR}{(\mu_0 H_0 \pi a)^2}.$$

The electrical resistance is:

$$R = \frac{2\pi a}{\sigma A},$$

with A the cross section of the wire that forms the ring. On the other hand, the mass of the ring is:

$$m = 2\pi a A \rho.$$

Then:

$$mR = \frac{\rho}{\sigma} (2\pi a)^2.$$

Hence τ becomes:

$$\tau = \frac{4\rho}{\mu_0^2 H_0^2 \sigma} = 1.5 \text{ s}.$$

4 Quantum Control

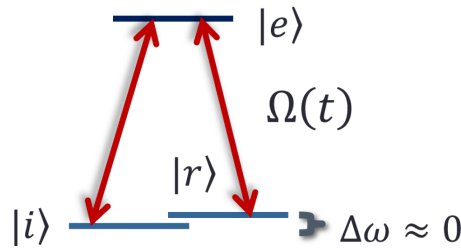


Figure 5: Sketch of the three-level system considered in the problem.

Quantum control is the field that studies how to manipulate quantum systems to optimize quantum processes. We want to control transitions between the initial, intermediate, and final states ($|i\rangle$, $|e\rangle$, and $|r\rangle$, respectively), as shown in Fig. 5. In resonant conditions, when the photon frequency matches the energy difference between the excited $|e\rangle$ and initial $|i\rangle$ state, and the energy difference between the $|i\rangle$ and $|r\rangle$ states is small ($\hbar\Delta\omega \approx 0$), a single laser pulse $\mathcal{E}(t)$ can drive both transitions $|i\rangle \rightarrow |e\rangle$ and $|e\rangle \rightarrow |r\rangle$ (typically referred to as the Rayleigh-Raman line).

Under very general approximations, we can write the Hamiltonian in the interaction picture as

$$\hat{H}(t) = -\frac{\Omega(t)}{2} \left(|i\rangle\langle e| + |e\rangle\langle i| + |e\rangle\langle r| + |r\rangle\langle e| \right),$$

where $\Omega(t) = \mu\mathcal{E}(t)/\hbar$, the so-called Rabi frequency, represents the coherent interaction between the field and the system. The time-dependent Schrödinger equation (TDSE) can be solved analytically, with time-evolution operator mapped onto the matrix (with the implicit basis order: $|i\rangle, |e\rangle, |r\rangle$):

$$U(t, 0) \doteq \begin{pmatrix} \frac{\cos\theta(t) + 1}{2} & \frac{i \sin\theta(t)}{\sqrt{2}} & \frac{\cos\theta(t) - 1}{2} \\ \frac{i \sin\theta(t)}{\sqrt{2}} & \cos\theta(t) & \frac{i \sin\theta(t)}{\sqrt{2}} \\ \frac{\cos\theta(t) - 1}{2} & \frac{i \sin\theta(t)}{\sqrt{2}} & \frac{\cos\theta(t) + 1}{2} \end{pmatrix},$$

where $\theta(t) = \int_0^t \Omega(t') dt' / \sqrt{2}$ is the mixing angle of the superposition state that is being formed. After the pulse is switched off, the pulse integral or pulse area, $A \equiv \int_0^\infty \Omega(t) dt = \sqrt{2}\theta(\infty)$, is the only external parameter that controls the final state of the system.

1. **(4 points)** Proof that $U(t, 0)$ is the solution of the TDSE. Consider units of $\hbar = 1$.
2. **(1.5 points)** Calculate the maximum value for the transition probability from state $|r\rangle$ to state $|i\rangle$. What values of A maximize the probability? This choice represents maximizing the yield of the Raman transition.
3. **(1.5 points)** Calculate the maximum value for the transition probability from state $|e\rangle$ to state $|i\rangle$. What values of A maximize the probability? This choice represents maximizing the yield of the electronic absorption.
4. **(3 points)** Find the initial state $|\psi\rangle_0 = c_i |i\rangle + c_r |r\rangle$ that should be prepared in order to reach $|e\rangle$ with certainty or with null probability (either maximum control or transparency, respectively).

Solutions

1. (4 points) Proof that the given $U(t, 0)$ is the solution of the TDSE. Consider units of $\hbar = 1$.

The time-evolution operator is defined through its action on the wave function, $|\Psi\rangle_t = \hat{U}(t, 0) |\Psi\rangle_0$. From the TDSE, $\partial_t |\Psi\rangle_t = -i\hat{H}(t) |\Psi\rangle_t$ (using units with $\hbar = 1$), it follows that $\partial_t \hat{U}(t, 0) = -i\hat{H}(t)\hat{U}(t, 0)$. In matrix form, deriving $\partial_t U(t, 0)$ (with $\dot{\theta} = \Omega(t)/\sqrt{2}$) we find

$$\partial_t U(t, 0) = \frac{\Omega(t)}{\sqrt{2}} \begin{pmatrix} -\sin \theta/2 & i \cos \theta/\sqrt{2} & \sin \theta/2 \\ i \cos \theta/\sqrt{2} & -\sin \theta & i \cos \theta/\sqrt{2} \\ -\sin \theta/2 & i \cos \theta/\sqrt{2} & \sin \theta/2 \end{pmatrix}.$$

In the basis $\{|i\rangle, |e\rangle, |r\rangle\}$, the Hamiltonian can be written as

$$\hat{H} \doteq H = -\frac{1}{2}\Omega(t) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Then

$$-iH(t)U(t, 0) = \frac{i}{2}\Omega(t) \begin{pmatrix} i \sin \theta/\sqrt{2} & \cos \theta & i \sin \theta/\sqrt{2} \\ \cos \theta & i\sqrt{2} \sin \theta & \cos \theta \\ i \sin \theta/\sqrt{2} & \cos \theta & i \sin \theta/\sqrt{2} \end{pmatrix},$$

which is identical to $\partial_t U(t, 0)$.

2. (1.5 points) Calculate the maximum value for the transition probability from state $|r\rangle$ to state $|i\rangle$. What values of A maximize the probability? This choice represents maximizing the yield of the Raman transition.

The probability to reach $|r\rangle$ from $|i\rangle$ at final time is given by the complex square of the matrix element U_{31} , as $P(\infty) = U_{31}^* U_{31} = [\cos \theta(\infty) - 1]^2 / 4 = \sin^4(\theta(\infty)/2)$. It is therefore possible to reach state $|r\rangle$ with certainty if $\theta(\infty)/2 = A/(2\sqrt{2}) = (2n + 1)\pi/2$, with $n \in \mathbb{Z}$. Maximum population transfer requires the pulse area to be $A = \sqrt{2}(2n + 1)\pi$, with $n \in \mathbb{Z}$.

3. (1.5 points) Calculate the maximum value for the transition probability from state $|e\rangle$ to state $|i\rangle$. What values of A maximize the probability? This choice represents maximizing the yield of the electronic absorption.

The probability to reach $|e\rangle$ from $|i\rangle$ at final time is given by the complex square of the matrix element U_{21} , as $P(\infty) = U_{21}^* U_{21} = [\sin \theta(\infty)]^2 / 2$. A maximum probability of 50% can be achieved when $\theta(\infty) = A/\sqrt{2} = (2n + 1)\pi/2$, with $n \in \mathbb{Z}$, for which $A = (2n + 1)\pi/\sqrt{2}$, with $n \in \mathbb{Z}$.

4. (3 points) Find which initial state $|\psi\rangle_0 = c_i |i\rangle + c_r |r\rangle$ must be prepared such that one can reach state $|e\rangle$ with certainty or with null probability (either maximum control or transparency, respectively).

To reach state $|r\rangle$ with certainty from a superposition of $|i\rangle$ and $|r\rangle$, we need

$$U \begin{pmatrix} c_i \\ 0 \\ c_r \end{pmatrix} = \begin{pmatrix} 0 \\ z \\ 0 \end{pmatrix},$$

where z is a complex number of modulo 1. Then, $z = U_{21}c_i + U_{23}c_r = i \sin \theta(\infty)(c_i + c_r)/\sqrt{2}$ and

$$z^* z = \frac{1}{2} \sin^2 \theta(\infty) [|c_i|^2 + |c_r|^2 + 2\text{Re}(c_i c_r)] = 1,$$

for which we need to make $\sin^2 \theta(\infty) = 1$ and $[|c_i|^2 + |c_r|^2 + 2\text{Re}(c_i c_r)] = 2$. The first condition requires, as in the previous case, that $A = (2n + 1)\pi/\sqrt{2}$, with $n \in \mathbb{Z}$. The latter is only possible if we have maximum constructive interference, that is, $\text{Re}(c_i c_r) = 1/2$. This forces $c_i = c_r = e^{i\alpha}/\sqrt{2}$. We need to prepare initially the totally symmetric superposition. Then, the term in the square parenthesis is equal to 2, and $z^* z = 1$.

To achieve transparency conditions, we need to cancel the transfer probability (destructive interference), for which $z = \mathbf{U}_{21}c_i + \mathbf{U}_{23}c_r = i \sin \theta(\infty)(c_i + c_r)/\sqrt{2} = 0$. We thus need $c_r = -c_i$.

Alternatively, we can find conditions where $\sin^2 \theta(\infty) = 0$, for which $\theta(\infty) = n\pi$ and hence $A = \sqrt{2}n\pi$, with $n \in \mathbb{Z}$, regardless of the initial state. This is an obvious solution because, e.g. if we do not use a laser ($A = 0$), the system can not leave the initial state. However, by preparing the superposition state $|\psi\rangle_0 = (|i\rangle - |r\rangle)/\sqrt{2}$ we can guarantee that the system will not be excited, regardless of the pulse features.

5 Solid State Physics

The electronic band structure in solids is related to the quantum states of an electron in a periodic potential. The electron wave function corresponding to an eigenstate, $\psi(\vec{r})$, must satisfy the Bloch theorem, i.e.,

$$\psi(\vec{r}) \sim e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r}),$$

where $u_{\vec{k}}(\vec{r})$ is a periodic function, i.e., $u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r})$, where \vec{R} is a lattice vector.

A simple one-dimensional model to describe electron states in a periodic potential corresponds to approximate the potential $U(x)$ by

$$U(x) = \sum_{n=-\infty}^{\infty} aV_0\delta(x + na),$$

where a is the lattice parameter.

1. **(4 points)** Demonstrate that the dispersion relation between the energy levels ϵ and the wavevector k is given by

$$\cos ka = \frac{\kappa}{q} \sin qa + \cos qa,$$

where $\epsilon = \hbar^2 q^2 / 2m$ and $\kappa = \alpha V_0$. Determine the coefficient α .

2. **(2 points)** In the low energy limit, demonstrate that

$$\epsilon(k) = E_0 + \frac{\hbar^2 k^2}{2m^*},$$

where m^* can be considered as the electron *effective mass* in the presence of the periodic potential. Obtain an expression for m^* in this limit, and verify that it can be bigger, smaller or equal to m .

3. **(2 points)** Calculate the *gaps* between the energy bands assuming that $V_0 \ll \hbar^2/ma^2$ (weak potential limit).
4. **(2 points)** Calculate the bandwidth corresponding to the lowest band in the limit $V_0 \gg \hbar^2/ma^2$.

Solutions

1. (4 points) Demonstrate that the dispersion relation between the energy levels ϵ and the wavevector k is given by

$$\cos ka = \frac{\kappa}{q} \sin qa + \cos qa,$$

where $\epsilon = \hbar^2 q^2 / 2m$ and $\kappa = \alpha V_0$. Determine the coefficient α .

The general solution is of the form

$$\psi(x) = A\psi_{\text{right}}(x) + B\psi_{\text{left}}(x),$$

where

$$\psi_{\text{left}}(x) = \begin{cases} e^{iqx} + re^{-iqx}, & x \leq 0 \\ te^{iqx}, & x > 0 \end{cases},$$

and

$$\psi_{\text{right}}(x) = \begin{cases} te^{-iqx}, & x \leq 0 \\ e^{-iqx} + re^{iqx}, & x > 0 \end{cases},$$

where the state energy ϵ is set by $\hbar^2 q^2 / 2m$. Imposing Bloch's theorem,

$$\begin{aligned} \psi(x+a) &= e^{ika} \psi(x), \\ \frac{d\psi}{dx}(x+a) &= e^{ika} \frac{d\psi}{dx}(x). \end{aligned}$$

Evaluating these two equations at $x = -a/2$ one obtains two homogeneous equations. The condition for a non trivial solution yields

$$\cos ka = \frac{1}{2t} e^{-iqa} + \left(\frac{t^2 - r^2}{2t} \right) e^{iqa}.$$

We now need to solve for t and r for a delta-like potential. Imposing continuity of the wavefunction at $x = 0$ and discontinuity of the derivative due to the delta potential, we obtain

$$\begin{aligned} r &= \frac{\kappa}{iq - \kappa}, \\ t &= \frac{iq}{iq - \kappa}, \end{aligned}$$

where $\kappa = mV_0a/\hbar^2$. Substituting in the dispersion relation, we finally obtain

$$\cos ka = \cos qa + \frac{\kappa}{q} \sin qa.$$

2. (2 points) In the low energy limit, demonstrate that

$$\epsilon(k) = E_0 + \frac{\hbar^2 k^2}{2m^*},$$

where m^* can be considered as the electron *effective mass* in the presence of the periodic potential. Obtain an expression for m^* in this limit, and verify that it can be bigger, smaller or equal to m .

We need to consider ϵ , q , and $k \rightarrow 0$. In this limit, we can consider the approximations $\sin qa \approx qa - (qa)^3/6$, $\cos qa \approx 1 - (qa)^2/2$, and $\cos ka \approx 1 - (ka)^2/2$. Then, substituting

these approximations in the last equation of question 1, and grouping terms in q^2 , we can express $\epsilon = \hbar^2 q^2 / 2m$ as

$$\epsilon = \frac{\hbar^2 k^2}{2m^*} + E_0,$$

where

$$m^* = m \left(\frac{\kappa a}{3} + 1 \right),$$

$$E_0 = \frac{\hbar^2}{ma^2} \left(\frac{\kappa a}{3} + 1 \right).$$

This result shows that m^* can be larger or smaller than m depending on the sign of V_0 .

3. **(2 points)** Calculate the *gaps* between the energy bands assuming that $V_0 \ll \hbar^2/ma^2$ (weak potential limit).

The band limits correspond to $\cos ka = (-1)^m$,

$$\cos qa + \frac{\kappa}{q} \sin qa = \pm 1.$$

The crossing points can be denoted by $qa = m\pi + \delta$, with $\delta \ll 1$ in the limit $V_0 \rightarrow 0$. We thus get

$$\cos \delta + \frac{\kappa}{q} \sin \delta = 1.$$

In the large V_0 limit, $\delta \rightarrow 0$ and we get $\delta \simeq 2\kappa a / \pi m$. Then, we can get the gap energy $\Delta\epsilon$ from

$$\Delta\epsilon = \epsilon \left(q = \frac{m\pi}{a} + \frac{\delta}{a} \right) - \epsilon \left(q = \frac{m\pi}{a} \right),$$

which yields

$$\Delta\epsilon \sim 2V_0.$$

4. **(2 points)** Calculate the bandwidth corresponding to the lowest band in the limit $V_0 \gg \hbar^2/ma^2$.

If $V_0 \gg \hbar^2/ma^2$, we have $\kappa a \gg 1$. The first band extends from the crossing at positive energy E_0 and the crossing E_1 . This last one corresponds to $qa = \pi$, so that $E_1 = -\hbar^2/2m(\pi/a)^2$. The value of q at E_0 is set by

$$1 = \cos q_0 a + \frac{\kappa}{q_0} \sin q_0 a,$$

so that

$$\frac{\kappa}{q_0} = \tan \left(\frac{q_0 a}{2} \right).$$

In the limit $\kappa a \rightarrow \infty$, $q_0 a \rightarrow \pi$ so that $q_0 a / 2 \simeq (\pi - \delta) / 2$, with $\delta \ll 1$. We get $\delta \simeq 2q_0 / \kappa$, so that $q_0 \simeq \pi \kappa / (a\kappa + 2)$. Then

$$\Delta\epsilon = E_1 - E_0 \simeq \frac{2\hbar^2 \pi^2}{ma^2} \left(\frac{1}{\kappa a} \right).$$

6 Quantum Optics

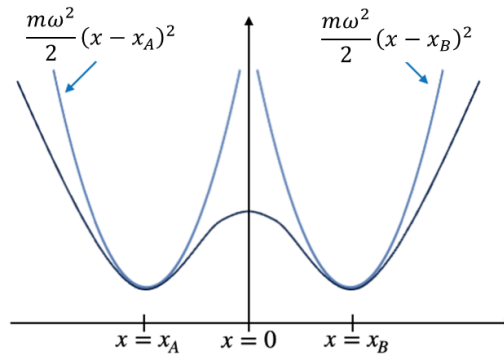


Figure 6: Sketch of the potential energy curve of a 1D molecule.

We assume one electron in a molecule formed by two atoms A and B with a potential energy as given in Fig. 6, where $x_A = -x_B$. We simplify the molecular potential by doing a Taylor expansion around the atomic sites x_A and x_B . Hence, the Hamiltonian of the electron is reduced to

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}(x - x_A)^2 + \frac{m\omega^2}{2}(x - x_B)^2.$$

- (2 points) Show that the delocalized states described by the wavefunctions

$$\begin{aligned}\psi_0(x) &= \frac{1}{\sqrt{2}} [\psi_A(x) + \psi_B(x)], \\ \psi_1(x) &= \frac{1}{\sqrt{2}} [\psi_A(x) - \psi_B(x)],\end{aligned}$$

are eigenstates with energy $E_0 = \hbar\omega/2$. Note that $\{\psi_A(x), \psi_B(x)\}$ are the atomic ground-state wavefunctions at sites A and B, respectively.

Hint: You may consider that the wavefunctions at the two atomic sites are well localized, and do not overlap with the other site. Also, remember the quantum harmonic oscillator solution:

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}(x - x_i)^2 \right] \psi_i(x) = E_0 \psi_i(x),$$

where

$$\psi_i(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar}(x-x_i)^2},$$

with eigenenergy $E_0 = \hbar\omega/2$.

- (2 points) Now we apply a time-varying electric field $\mathcal{E}(t) = \mathcal{E}_0 \cos \omega t$ to the molecule. The interaction Hamiltonian with the molecule is described by $\hat{V}_I(t) = e\hat{x}\mathcal{E}(t)$, where e and x are the charge and the position of the electron, respectively. Calculate the transition elements:

$$\langle \psi_A | \hat{x} | \psi_A \rangle, \quad \langle \psi_A | \hat{x} | \psi_B \rangle, \quad \langle \psi_B | \hat{x} | \psi_A \rangle, \quad \text{and} \quad \langle \psi_B | \hat{x} | \psi_B \rangle.$$

Construct the matrix in the basis $\{\psi_A(x), \psi_B(x)\}$ representing the total hamiltonian, i.e., the matrix with elements $(H_{AB})_{ij} \equiv \langle i | [\hat{H} + \hat{V}_I(t)] | j \rangle$.

3. (4 points) During the time-varying electric field, we consider the time-dependent state as a superposition of our atomic basis as $|\psi(t)\rangle = a(t)|\psi_A\rangle + b(t)|\psi_B\rangle$, where $a(t)$ and $b(t)$ are complex amplitudes. Find the form of $a(t)$ and $b(t)$ if we know that at $t = 0$ the state is in the delocalized state $|\psi(t = 0)\rangle = |\psi_0\rangle = (|\psi_A\rangle + |\psi_B\rangle)/\sqrt{2}$.

Hint: The electron state evolves following $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}_{AB}(t)|\psi(t)\rangle$, with solution given by $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt' \hat{H}_{AB}(t')}|\psi(t = 0)\rangle$. This choice represents maximizing the yield of the electronic absorption.

4. (2 points) The evolving state depends on the frequency of the electric field $\omega = 2\pi/\tau$, where τ is the period of this field. Find the vector potential amplitude $A_0 = \mathcal{E}_0/\omega$, such that, after a quarter of a period, the initial state $|\psi_0\rangle = (|\psi_A\rangle + |\psi_B\rangle)/\sqrt{2}$ transforms into $|\psi_1\rangle = (|\psi_A\rangle - |\psi_B\rangle)/\sqrt{2}$ (up to a global phase factor).

Solutions

1. (2 points) Show that the delocalized states described by the wavefunctions

$$\begin{aligned}\psi_0(x) &= \frac{1}{\sqrt{2}} [\psi_A(x) + \psi_B(x)], \\ \psi_1(x) &= \frac{1}{\sqrt{2}} [\psi_A(x) - \psi_B(x)],\end{aligned}$$

are eigenstates with energy $E_0 = \hbar\omega/2$. Note that $\{\psi_A(x), \psi_B(x)\}$ are the atomic ground-state wavefunctions at sites A and B , respectively.

We apply first the Hamiltonian operator to the atomic wavefunctions $\{\psi_A(x), \psi_B(x)\}$,

$$\begin{aligned}\hat{H}\psi_A(x) &= \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}(x-x_A)^2 + \frac{m\omega^2}{2}(x-x_B)^2 \right] \psi_A(x) \\ &\approx \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega^2}{2}(x-x_A)^2 \right] \psi_A(x) \\ &= E_0\psi_A(x),\end{aligned}$$

where we approximate that the wavefunction $\psi_A(x)$ is negligible at the B site. We have then a quantum harmonic oscillator. We can do the same for $\psi_B(x)$. Therefore,

$$\hat{H}\psi_{0,1}(x) = \hat{H} \frac{1}{\sqrt{2}} [\psi_A(x) \pm \psi_B(x)] \approx E_0 \frac{1}{\sqrt{2}} [\psi_A(x) \pm \psi_B(x)] = E_0\psi_{0,1}(x).$$

2. (2 points) Now we apply a time-varying electric field $\mathcal{E}(t) = \mathcal{E}_0 \cos \omega t$ to the molecule. The interaction Hamiltonian with the molecule is described by $\hat{V}_I(t) = e\hat{x}\mathcal{E}(t)$, where e and x are the charge and the position of the electron, respectively. Calculate the transition elements:

$$\langle \psi_A | \hat{x} | \psi_A \rangle, \quad \langle \psi_A | \hat{x} | \psi_B \rangle, \quad \langle \psi_B | \hat{x} | \psi_A \rangle, \quad \text{and} \quad \langle \psi_B | \hat{x} | \psi_B \rangle.$$

Construct the matrix in the basis $\{\psi_A(x), \psi_B(x)\}$ representing the total hamiltonian, i.e., the matrix with elements $(H_{AB})_{ij} \equiv \langle i | [\hat{H} + \hat{V}_I(t)] | j \rangle$.

We define $\alpha \equiv (m\omega/\pi\hbar)^{1/4}$ and $\beta \equiv m\omega/2\hbar$. Then

$$\langle \psi_A | \hat{x} | \psi_A \rangle = \alpha^2 \int_{-\infty}^{\infty} dx e^{-2\beta(x-x_A)^2} x = \alpha^2 \int_{-\infty}^{\infty} dx e^{-2\beta(x-x_A)^2} (x - x_A + x_A).$$

Because $e^{-2\beta(x-x_A)^2}$ and $(x - x_A)$ have different parity, the integral of these two terms is zero. The only remaining one is

$$\langle \psi_A | \hat{x} | \psi_A \rangle = \alpha^2 \int_{-\infty}^{\infty} dx e^{-2\beta(x-x_A)^2} x_A = x_A,$$

where we use the orthonormality of the wavefunction $\psi_A(x)$. Analogously, $\langle \psi_B | \hat{x} | \psi_B \rangle = x_B$. Now,

$$\begin{aligned}\langle \psi_A | \hat{x} | \psi_B \rangle &= \alpha^2 \int_{-\infty}^{\infty} dx e^{-\beta(x-x_A)^2} x e^{-\beta(x-x_B)^2} \\ &= \alpha^2 \int_{-\infty}^{\infty} dx e^{-\beta(2x^2 - 2x(x_A+x_B) + x_A^2 + x_B^2)} x \\ &= \alpha^2 e^{-\beta(x_A^2 + x_B^2)} \int_{-\infty}^{\infty} dx e^{-2\beta x^2} x = 0,\end{aligned}$$

which is also zero for parity reasons. Analogously, $\langle \psi_B | \hat{x} | \psi_A \rangle = 0$. Therefore, the matrix H_{AB} is

$$H_{AB} = \begin{pmatrix} \langle \psi_A | [\hat{H} + \hat{V}_I(t)] | \psi_A \rangle & \langle \psi_A | [\hat{H} + \hat{V}_I(t)] | \psi_B \rangle \\ \langle \psi_B | [\hat{H} + \hat{V}_I(t)] | \psi_A \rangle & \langle \psi_B | [\hat{H} + \hat{V}_I(t)] | \psi_B \rangle \end{pmatrix} = \begin{pmatrix} E_0 + ex_A \mathcal{E}(t) & 0 \\ 0 & E_0 + ex_B \mathcal{E}(t) \end{pmatrix}.$$

3. **(4 points)** During the time-varying electric field, we consider the time-dependent state as a superposition of our atomic basis as $|\psi(t)\rangle = a(t)|\psi_A\rangle + b(t)|\psi_B\rangle$, where $a(t)$ and $b(t)$ are complex amplitudes. Find the form of $a(t)$ and $b(t)$ if we know that at $t = 0$ the state is in the delocalized state $|\psi(t=0)\rangle = |\psi_0\rangle = (|\psi_A\rangle + |\psi_B\rangle)/\sqrt{2}$.

The time-evolved state is

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{i}{\hbar} \int_0^t dt' \hat{H}_{AB}(t')} |\psi(t=0)\rangle \\ &= \frac{1}{\sqrt{2}} \left[e^{-\frac{i}{\hbar} \int_0^t dt' \hat{H}_{AB}(t')} |\psi_A\rangle + e^{-\frac{i}{\hbar} \int_0^t dt' \hat{H}_{AB}(t')} |\psi_B\rangle \right]. \end{aligned}$$

Because $\{|\psi_A\rangle, |\psi_B\rangle\}$ are eigenstates of the matrix H_{AB} , with eigenvalues $\{E_0 + ex_A \mathcal{E}(t), E_0 + ex_B \mathcal{E}(t)\}$, the exponential of the matrix is the exponential of the eigenvalue, and then

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{2}} \left\{ e^{-\frac{i}{\hbar} \int_0^t dt' [E_0 + ex_A \mathcal{E}(t')] } |\psi_A\rangle + e^{-\frac{i}{\hbar} \int_0^t dt' [E_0 + ex_B \mathcal{E}(t')] } |\psi_B\rangle \right\} \\ &= \frac{1}{\sqrt{2}} \left[e^{-\frac{i}{\hbar} (E_0 t + ex_A \mathcal{E}_0 \sin \omega t / \omega)} |\psi_A\rangle + e^{-\frac{i}{\hbar} (E_0 t + ex_B \mathcal{E}_0 \sin \omega t / \omega)} |\psi_B\rangle \right] \\ &= a(t) |\psi_A\rangle + b(t) |\psi_B\rangle, \end{aligned}$$

from which we obtain the form for $a(t)$ and $b(t)$:

$$\begin{aligned} a(t) &= \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar} (E_0 t + ex_A \mathcal{E}_0 \sin \omega t / \omega)}, \\ b(t) &= \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar} (E_0 t + ex_B \mathcal{E}_0 \sin \omega t / \omega)}. \end{aligned}$$

4. **(2 points)** The evolving state depends on the frequency of the electric field $\omega = 2\pi/\tau$, where τ is the period of this field. Find the vector potential amplitude $A_0 = \mathcal{E}_0/\omega$, such that, after a quarter of a period, the initial state $|\psi_0\rangle = (|\psi_A\rangle + |\psi_B\rangle)/\sqrt{2}$ transforms into $|\psi_1\rangle = (|\psi_A\rangle - |\psi_B\rangle)/\sqrt{2}$ (up to a global phase factor).

Starting from the calculated time-dependent state $|\psi(t)\rangle$, we factorize the global phase factor

$$e^{-\frac{i}{\hbar} (E_0 t + ex_A \mathcal{E}_0 \sin \omega t / \omega)},$$

which renders

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar} (E_0 t + ex_A \mathcal{E}_0 \sin \omega t / \omega)} \left[|\psi_A\rangle + e^{-ie(x_B - x_A)\mathcal{E}_0 \sin \omega t / \hbar \omega} |\psi_B\rangle \right].$$

When $t = \tau/4$, we need the relative phase to be equal to π , i.e.,

$$-\frac{e\mathcal{E}_0}{\hbar\omega} (x_B - x_A) \sin\left(\frac{\omega\tau}{4}\right) = \frac{2ex_A \mathcal{E}_0}{\hbar\omega} \sin\left(\frac{\omega\tau}{4}\right) = \pi,$$

in order to obtain $e^{i\pi} = -1$. This is satisfied when

$$A_0 = \frac{\mathcal{E}_0}{\omega} = \frac{\pi\hbar}{2ex_A}.$$

7 Quantum Information

A finite-dimensional quantum system S is prepared in either state ρ_1 with probability p or state ρ_2 with probability $1 - p$.

1. **(3 points)** What is the maximum average probability $P_{\max}(p, \rho_1, \rho_2)$ of correctly guessing the state of this system using only a single measurement run?
2. **(4 points)** Prove that a trace-preserving (and Hermitian-preserving) map \mathcal{E} is a quantum channel if and only if

$$P_{\max}(p, \sigma_1, \sigma_2) \geq P_{\max}[p, \mathcal{E} \otimes \mathbb{I}(\sigma_1), \mathcal{E} \otimes \mathbb{I}(\sigma_2)],$$

for all $p \in [0, 1]$ and for any pair σ_1 and σ_2 of density matrices corresponding to a system composed of two copies of S .

3. **(3 points)** If $\rho_1 = \frac{1}{4}(3|+\rangle\langle+| + |-\rangle\langle-|)$ and $\rho_2 = |0\rangle\langle 0|$ with $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ and $\{|0\rangle, |1\rangle\}$ forms an orthonormal basis of a qubit system, find the value of p that minimizes $P_{\max}(p, \rho_1, \rho_2)$.

Solutions

1. (3 points) What is the maximum average probability $P_{\max}(p, \rho_1, \rho_2)$ of correctly guessing the state of this system using only a single measurement run?

To distinguish between ρ_1 and ρ_2 , we can divide the set of measurement outcomes \mathcal{X} of a general POVM $\{x, E_x\}_{x \in \mathcal{X}}$ into two complementary subsets $\mathcal{X}_1 \subset \mathcal{X}$ and $\mathcal{X}_2 \subset \mathcal{X}$, satisfying $\mathcal{X}_1 \cup \mathcal{X}_2 = \mathcal{X}$ and $\mathcal{X}_1 \cap \mathcal{X}_2 = \emptyset$. If the measurement result belongs to \mathcal{X}_1 , we identify the system state as ρ_1 , and if it belongs to \mathcal{X}_2 , we identify it as ρ_2 .

Thus, for the purpose of distinguishing between ρ_1 and ρ_2 , any POVM $\{x, E_x\}_{x \in \mathcal{X}}$ is equivalent to another measurement $\{n, T_n\}_{n=1}^2$, with $T_{1,2} = \sum_{x \in \mathcal{X}_{1,2}} E_x$. Actually, by calling $T := T_1$, then $T_2 = \mathbb{I} - T$.

Now, when the true state of the system is ρ_1 , the state is correctly identified with probability

$$\sum_{x \in \mathcal{X}_1} P(x|\rho_1) = \sum_{x \in \mathcal{X}_1} \text{Tr}[\rho_1 E_x] = \text{Tr} \left[\rho_1 \left(\sum_{x \in \mathcal{X}_1} E_x \right) \right] = \text{Tr}(\rho_1 T).$$

Similarly, when the true state is ρ_2 , the state is correctly identified with probability

$$\sum_{x \in \mathcal{X}_2} P(x|\rho_2) = \sum_{x \in \mathcal{X}_2} \text{Tr}[\rho_2 E_x] = \text{Tr} \left[\rho_2 \left(\sum_{x \in \mathcal{X}_2} E_x \right) \right] = \text{Tr}[\rho_2(\mathbb{I} - T)].$$

Therefore, the maximum averaged probability of correctly guessing the state is

$$\begin{aligned} P_{\max}(p, \rho_1, \rho_2) &= \max_{0 \leq T \leq \mathbb{I}} \{p \text{Tr}(\rho_1 T) + (1-p) \text{Tr}[\rho_2(\mathbb{I} - T)]\} \\ &= (1-p) + \max_{0 \leq T \leq \mathbb{I}} \text{Tr}(\Delta T), \end{aligned}$$

with $\Delta = p\rho_1 - (1-p)\rho_2$. Now, using the spectral decomposition of this operator

$$\Delta = \sum_{j=1}^d \lambda_j |\psi_j\rangle\langle\psi_j|,$$

we obtain

$$P_{\max}(p, \rho_1, \rho_2) = (1-p) + \max_{0 \leq T \leq \mathbb{I}} \sum_j \lambda_j \langle\psi_j|T|\psi_j\rangle.$$

The condition $0 \leq T \leq \mathbb{I}$ reads

$$0 \leq \langle\psi|T|\psi\rangle \leq \langle\psi|\psi\rangle,$$

and so the maximum probability is achieved when T is a projection onto the subspace spanned by the eigenvectors associated with the positive eigenvalues of Δ . By ordering them so that these positive eigenvalues correspond to the first q in the labeling of j , we have $T = \sum_{j=1}^q |\psi_j\rangle\langle\psi_j|$,

$$\max_{0 \leq T \leq \mathbb{I}} \sum_j \lambda_j \langle\psi_j|T|\psi_j\rangle = \sum_{j=1}^q \lambda_j,$$

and

$$P_{\max}(p, \rho_1, \rho_2) = (1-p) + \sum_{j=1}^q \lambda_j.$$

Additionally, we can express this result using the trace norm. To this end, taking into account that

$$\sum_{j=1}^d \lambda_j = \text{Tr}(\Delta) = 2p - 1 \Rightarrow (1 - p) = \frac{1}{2} \left(1 - \sum_{j=1}^d \lambda_j \right),$$

we obtain

$$P_{\max}(p, \rho_1, \rho_2) = \frac{1}{2} - \frac{1}{2} \sum_{j=1}^d \lambda_j + \sum_{j=1}^q \lambda_j = \frac{1}{2} \left(1 + \sum_{j=1}^d |\lambda_j| \right) = \frac{1 + \|\Delta\|_1}{2},$$

where the trace norm $\|\Delta\|_1 := \sqrt{\Delta^\dagger \Delta} = \sum_{j=1}^d |\lambda_j|$ has been introduced.

2. **(4 points)** Prove that a trace-preserving (and Hermitian-preserving) map \mathcal{E} is a quantum channel if and only if

$$P_{\max}(p, \sigma_1, \sigma_2) \geq P_{\max}[p, \mathcal{E} \otimes \mathbb{I}(\sigma_1), \mathcal{E} \otimes \mathbb{I}(\sigma_2)],$$

for all $p \in [0, 1]$ and for any pair σ_1 and σ_2 of density matrices corresponding to a system composed of two copies of S .

According to the previous result, we have

$$P_{\max}(p, \sigma_1, \sigma_2) = \frac{1 + \|\Delta'\|_1}{2},$$

where

$$\Delta' := p\sigma_1 - (1 - p)\sigma_2 = \sum_{j=1}^{d^2} \lambda'_j |\Psi_j\rangle\langle\Psi_j|.$$

Alternatively, by again ordering the positive eigenvalues in increasing order (and assuming there are q' of them in this case), we obtain

$$P_{\max}(p, \sigma_1, \sigma_2) = (1 - p) + \sum_{j=1}^{q'} \lambda'_j.$$

First, consider that \mathcal{E} is a quantum channel, i.e., a completely positive and trace-preserving map, i.e., $\mathcal{E} \otimes \mathbb{I}$ maps density matrices to density matrices. Therefore,

$$P_{\max}[p, \mathcal{E} \otimes \mathbb{I}(\sigma_1), \mathcal{E} \otimes \mathbb{I}(\sigma_2)] = (1 - p) + \sum_{j=1}^r \mu_j,$$

where μ_j are the positive eigenvalues of $\mathcal{E} \otimes \mathbb{I}(\Delta')$, which are now ordered as the first r terms in the spectral decomposition

$$\mathcal{E} \otimes \mathbb{I}(\Delta') = \sum_{j=1}^{d^2} \mu_j |\Phi_j\rangle\langle\Phi_j|.$$

Thus, the maximum probability after the quantum channel can be rewritten as

$$P_{\max}[p, \mathcal{E} \otimes \mathbb{I}(\sigma_1), \mathcal{E} \otimes \mathbb{I}(\sigma_2)] = (1 - p) + \sum_{j=1}^r \langle\Phi_j|\mathcal{E} \otimes \mathbb{I}(\Delta')|\Phi_j\rangle.$$

Using the spectral decomposition again, we can split Δ' as the difference of two positive operators,

$$\Delta' = \sum_{j=1}^{q'} \lambda'_j |\Psi_j\rangle\langle\Psi_j| + \sum_{j=q'+1}^{d^2} \lambda'_j |\Psi_j\rangle\langle\Psi_j| = \Delta'_+ - \Delta'_-,$$

with

$$\begin{cases} \Delta'_+ = \sum_{j=1}^{q'} \lambda'_j |\Psi_j\rangle\langle\Psi_j|, \\ \Delta'_- = -\sum_{j=q'+1}^{d^2} \lambda'_j |\Psi_j\rangle\langle\Psi_j|. \end{cases}$$

We can then write

$$\begin{aligned} \sum_{j=1}^r \langle\Phi_j|\mathcal{E} \otimes \mathbb{I}(\Delta')|\Phi_j\rangle &= \sum_{j=1}^r \langle\Phi_j|\mathcal{E} \otimes \mathbb{I}(\Delta'_+)|\Phi_j\rangle - \sum_{j=1}^r \langle\Phi_j|\mathcal{E} \otimes \mathbb{I}(\Delta'_-)|\Phi_j\rangle \\ &\leq \sum_{j=1}^r \langle\Phi_j|\mathcal{E} \otimes \mathbb{I}(\Delta'_+)|\Phi_j\rangle \leq \sum_{j=1}^{d^2} \langle\Phi_j|\mathcal{E} \otimes \mathbb{I}(\Delta'_+)|\Phi_j\rangle \\ &= \text{Tr}[\mathcal{E} \otimes \mathbb{I}(\Delta'_+)] = \text{Tr}[\Delta'_+] = \sum_{j=1}^{q'} \lambda'_j. \end{aligned}$$

Here, we have used the facts that $\mathcal{E} \otimes \mathbb{I}(\Delta'_\pm)$ are positive operators (since Δ'_\pm are positive and $\mathcal{E} \otimes \mathbb{I}$ preserves positivity) and that $\mathcal{E} \otimes \mathbb{I}$ is trace-preserving. This proves

$$\mathbf{P}_{\max}(p, \sigma_1, \sigma_2) \geq \mathbf{P}_{\max}[p, \mathcal{E} \otimes \mathbb{I}(\sigma_1), \mathcal{E} \otimes \mathbb{I}(\sigma_2)],$$

for any p , σ_1 , and σ_2 , and for any quantum channel \mathcal{E} .

This inequality is expected from a physical point of view, since applying a quantum channel cannot increase the available information about the state of a system.

Conversely, if the inequality holds, we have

$$\|\mathcal{E} \otimes \mathbb{I}(\Delta')\|_1 \leq \|\Delta'\|_1,$$

for all Δ' . In particular, for $p = 1$, $\Delta' = \sigma_1$ is a density matrix, meaning it is a positive operator. Since the trace norm of a positive operator equals its trace, and $\mathcal{E} \otimes \mathbb{I}$ is trace-preserving, we obtain the following chain of inequalities:

$$\|\sigma_1\|_1 = \text{Tr}[\sigma_1] = \text{Tr}[\mathcal{E} \otimes \mathbb{I}(\sigma_1)] \leq \|\mathcal{E} \otimes \mathbb{I}(\sigma_1)\|_1 \leq \|\sigma_1\|_1.$$

Therefore,

$$\text{Tr}[\mathcal{E} \otimes \mathbb{I}(\sigma_1)] = \|\mathcal{E} \otimes \mathbb{I}(\sigma_1)\|_1,$$

and hence, $\mathcal{E} \otimes \mathbb{I}(\sigma_1)$ is positive for every positive operator σ_1 , meaning that \mathcal{E} is a completely positive and trace-preserving map.

3. **(3 points)** If $\rho_1 = \frac{1}{4}(3|+\rangle\langle+| + |-\rangle\langle-|)$ and $\rho_2 = |0\rangle\langle 0|$ with $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ and $\{|0\rangle, |1\rangle\}$ forms an orthonormal basis of a qubit system, find the value of p that minimizes $\mathbf{P}_{\max}(p, \rho_1, \rho_2)$.

In this case, we express Δ as a matrix in the basis $\{|0\rangle, |1\rangle\}$:

$$\Delta \equiv \frac{p}{4} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} - (1-p) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{3p}{2} - 1 & \frac{p}{4} \\ \frac{p}{4} & \frac{p}{2} \end{pmatrix}.$$

The eigenvalues of this matrix are given by

$$\lambda_{1,2}(p) = \frac{1}{4} \left(4p - 2 \pm \sqrt{5p^2 - 8p + 4} \right).$$

To determine when they vanish, we solve

$$\lambda_1 \lambda_2 = 0 \Rightarrow 11p^2 - 8p = 0 \Rightarrow p = 0, \frac{8}{11}.$$

The first solution, $p = 0$, causes the first eigenvalue to vanish: $\lambda_1(0) = 0$. The second solution, $p = \frac{8}{11}$, causes the second eigenvalue to vanish: $\lambda_2(\frac{8}{11}) = 0$. Since $\lambda_1(1) = \frac{3}{4}$, $\lambda_2(0) = -1$, and $\lambda_2(1) = \frac{1}{4}$, we conclude

$$\begin{aligned}\lambda_1(p) &\geq 0, & p \in [0, 1], \\ \lambda_2(p) &< 0, & p \in [0, \frac{8}{11}), \\ \lambda_2(p) &\geq 0, & p \in [\frac{8}{11}, 1].\end{aligned}$$

Thus, the maximum probability can be expressed as

$$P_{\max}(p, \rho_1, \rho_2) = \begin{cases} (1-p) + \lambda_1(p) = \frac{1}{4}(2 + \sqrt{5p^2 - 8p + 4}), & p \in [0, \frac{8}{11}], \\ (1-p) + \lambda_1(p) + \lambda_2(p) = p, & p \in [\frac{8}{11}, 1]. \end{cases}$$

The second-order polynomial $f(p) = 5p^2 - 8p + 4$ has a unique critical point at $p_0 = \frac{4}{5}$, which corresponds to a minimum:

$$\begin{aligned}f'(p) &= 10p - 8 = 0 \Rightarrow p = \frac{4}{5}, & f(\frac{4}{5}) &= \frac{4}{5}, \\ f''(p) &= 10 > 0.\end{aligned}$$

Since $p_0 > \frac{8}{11}$, the minimum value of $P_{\max}(p, \rho_1, \rho_2)$ for $p \in [0, \frac{8}{11}]$ occurs at $p = \frac{8}{11}$. Furthermore, the probability also attains its minimum at this point for $p \in [\frac{8}{11}, 1]$, so we conclude that the global minimum is attained at $p = \frac{8}{11}$.

8 Gravitational Waves

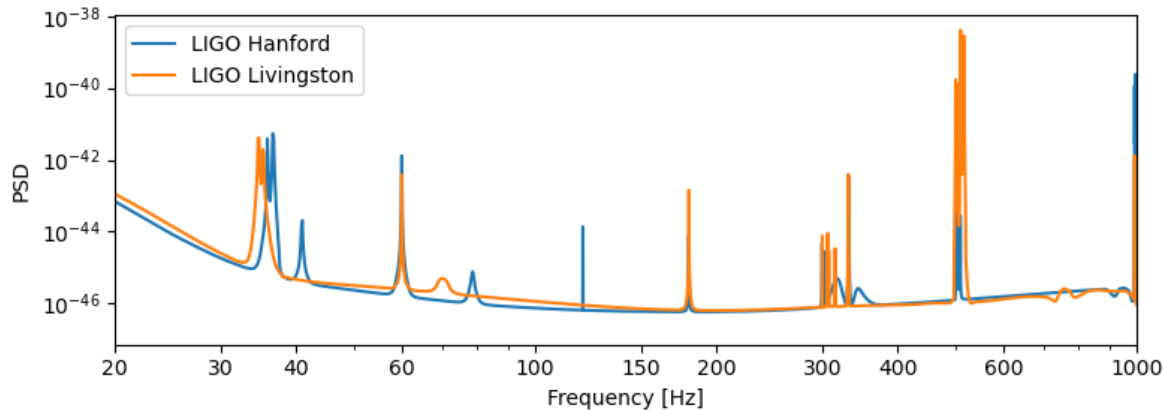


Figure 7: Power spectral density registered by the two LIGO interferometers after the detection of the GW150914 event in 2015.

Gravitational waves are produced by accelerating massive objects. For example, the groundbreaking detection of the GW150914 event ten years ago was supposed to be originated on a coalescing binary of two black holes of masses $m_1 = 36 M_\odot$ and $m_2 = 29 M_\odot$ at a distance $d = 410$ Mpc. The general expression of the gravitational strain $h(t, r)$ is

$$h(t, r) = \frac{h_0}{r} e^{i(\Omega t_r + \phi_0)},$$

where $h_0 \in \mathbb{R}, h_0 > 0$ is the strain amplitude, r is the distance between source and observer, Ω is the wave angular frequency, and $t_r = t - r/c$ is the retarded time.

Important: In the questions below, please, make sure that you include all the steps necessary to understand how you have obtained a given equation or expression whenever they will be required. Unjustified answers will only be partially considered.

- (1 point)** Consider a binary system with masses m_1 and m_2 in a circular orbit separated a distance R , and with center of mass at the origin $(0, 0)$. Obtain the positions $\vec{r}_1(t)$ and $\vec{r}_2(t)$ of the two objects provided the orbit is contained within the XY -plane and the orbital frequency is ω . Assume that both masses are initially ($t = 0$) along the x -axis, with the x -component of $\vec{r}_1(0)$ being $r_{1,x}(0) > 0$. Use $M \equiv m_1 + m_2$.
- (1 point)** By means of Newtonian mechanics, determine the expression of the angular orbital frequency ω in terms of M , R , and the gravitational constant G .
- (1.5 points)** Construct the gravitational wave tensor $\bar{h}_{ij}(t, r)$. To this end, note that, if the objects are slowly orbiting, the wave strain can be obtained in the weak-field limit by means of the quadrupole formula:

$$\bar{h}_{ij}(t, r) = \frac{2G}{c^4 r} \ddot{Q}_{ij}(t_r),$$

where $\bar{h}_{ij}(t, r)$ is the spatial part of the metric perturbation tensor at a time t and distance r to the source, c is the speed of light in free space, and $Q_{ij}(t)$ is the (transverse-traceless) mass-quadrupole moment tensor. The two upper dots in \ddot{Q}_{ij} denote the second derivative with

respect to time, and, for our configuration, the quadrupole tensor reads as

$$Q_{ij}(t) = \mu R^2 \begin{pmatrix} \cos^2 \omega t - \frac{1}{3} & \cos \omega t \sin \omega t & 0 \\ \cos \omega t \sin \omega t & \sin^2 \omega t - \frac{1}{3} & 0 \\ 0 & 0 & -\frac{1}{3} \end{pmatrix}$$

where i, j are the indices for the spatial components x, y, z , and $\mu = m_1 m_2 / M$ is the system reduced mass.

4. **(3 points)** Taking into account that the gravitational wave tensor obtained in question 3 can be recast as

$$\bar{h}_{ij}(t, r) = \begin{pmatrix} h_+ & h_\times & 0 \\ h_\times & -h_+ & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

where h_+ and h_\times are the gravitational wave polarizations, determine the expression for the gravitational wave strain $h(t, r) = h_+(t, r) + ih_\times(t, r)$, and, from it, provide the expressions for the strain amplitude h_0 and the wave angular frequency Ω . Substitute in the latter expressions the value of ω obtained in question 2. To get an idea of the orders of magnitude involved, provide the numerical value for both h_0 and Ω in the case of a binary black hole with $m_1 = m_2 = 30M_\odot$ separated a distance $R = 500$ km. Use $G = 6.7 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$, $M_\odot = 2 \times 10^{30} \text{ kg}$, and $c = 3 \times 10^8 \text{ m/s}$.

5. **(1 point)** Determine whether, for the frequency Ω corresponding to the example of binary system considered in question 4, the LIGO interferometers (see Fig. 7) are sensitive enough to the signals they emit.

Hint: The horizontal axis in Fig. 7 represents the range of frequencies $f = \Omega/2\pi$ at which the LIGO interferometers are sensitive. Specifically, the power spectral density baseline in both cases indicates the lowest spectral noise density (proportional to $|h_{\min}|^2$) detected at each frequency. The highest sensitivity is reached at about 175 Hz, for a spectral noise density of $\sim 10^{-46}$ and hence a minimum amplitude of $\sim 10^{-23}$.

6. **(1 point)** Assuming that the detection threshold is $|h| \gtrsim 10^{-21}$, how far away can the system be for it to still be detected? Express the distance in multiples of a parsec ($1 \text{ pc} = 3.1 \times 10^{16} \text{ m}$).
7. **(1.5 points)** Estimate the rate of binary black hole mergers in the universe taking into account that the first three rounds of observation of the LIGO Interferometers have had a combined duration of 448 days, and, in this time, 90 signals have been successfully identified. Express the rate in mergers/Gpc³·yr.

Hint: Assume all mergers behave like the system studied above.

Solutions

1. **(1 point)** Consider a binary system with masses m_1 and m_2 in a circular orbit separated a distance R , and with center of mass at the origin $(0, 0)$. Obtain the positions $\vec{r}_1(t)$ and $\vec{r}_2(t)$ of the two objects provided the orbit is contained within the XY -plane and the orbital frequency is ω . Assume that both masses are initially ($t = 0$) along the x -axis, with the x -component of $\vec{r}_1(0)$ being $r_{1,x}(0) > 0$. Use $M \equiv m_1 + m_2$.

We will assume m_1 starts at $\vec{r}_1(0) = (r_{1,x}, 0)$. Since it orbits around the origin, its position will be

$$\vec{r}_1(t) = \|\vec{r}_1\| (\cos \omega t, \sin \omega t),$$

Since the center of mass is $(0, 0)$, we have

$$m_1 \vec{r}_1(t) + m_2 \vec{r}_2(t) = 0 \Rightarrow \vec{r}_2(t) = -\frac{m_1}{m_2} \vec{r}_1(t).$$

To determine $r_1 = \|\vec{r}_1\|$ we impose that the separation is R at all times. Then,

$$\|\vec{r}_1 - \vec{r}_2\| = r_1 + \frac{m_1}{m_2} r_1 = R \Rightarrow r_1 = \frac{m_2 R}{M}.$$

So, putting it all together,

$$\begin{aligned} \vec{r}_1(t) &= \frac{m_2 R}{M} (\cos \omega t, \sin \omega t), \\ \vec{r}_2(t) &= -\frac{m_1 R}{M} (\cos \omega t, \sin \omega t). \end{aligned}$$

2. **(1 point)** By means of Newtonian mechanics, determine the expression of the angular orbital frequency ω in terms of M , R , and the gravitational constant G .

We consider the magnitude of the gravitational force

$$F_G = G \frac{m_1 m_2}{R^2},$$

and the centripetal force (of each mass with respect to the center of mass),

$$(F_c)_i = m_i a_i = m_i \omega^2 r_i = \frac{m_1 m_2}{M} R \omega^2 = \mu R \omega^2.$$

Equating the magnitudes of both forces leads to

$$F_G = F_c \Leftrightarrow G \frac{m_1 m_2}{R^2} = \frac{m_1 m_2}{M} R \omega^2 \Rightarrow \omega = \sqrt{\frac{GM}{R^3}}.$$

3. **(1.5 points)** Construct the gravitational wave tensor $\bar{h}_{ij}(t, r)$. To this end, note that, if the objects are slowly orbiting, the wave strain can be obtained in the weak-field limit by means of the quadrupole formula:

$$\bar{h}_{ij}(t, r) = \frac{2G}{c^4 r} \ddot{Q}_{ij}(t_r).$$

First of all, we differentiate Q_{ij} twice with respect to time:

$$\begin{aligned}\dot{Q}_{ij}(t) &= \mu R^2 \omega \begin{pmatrix} -2 \cos \omega t \sin \omega t & \cos^2 \omega t - \sin^2 \omega t & 0 \\ \cos^2 \omega t - \sin^2 \omega t & 2 \cos \omega t \sin \omega t & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ &= \mu R^2 \omega \begin{pmatrix} -\sin 2\omega t & \cos 2\omega t & 0 \\ \cos 2\omega t & \sin 2\omega t & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \ddot{Q}_{ij}(t) &= 2\mu R^2 \omega^2 \begin{pmatrix} -\cos 2\omega t & -\sin 2\omega t & 0 \\ -\sin 2\omega t & \cos 2\omega t & 0 \\ 0 & 0 & 0 \end{pmatrix}.\end{aligned}$$

Now, using the quadrupole formula,

$$\bar{h}_{ij}(t, r) = \frac{4G\mu R^2 \omega^2}{c^4 r} \begin{pmatrix} -\cos 2\omega t_r & -\sin 2\omega t_r & 0 \\ -\sin 2\omega t_r & \cos 2\omega t_r & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

4. **(3 points)** Taking into account that the gravitational wave tensor obtained in question 3 can be recast as

$$\bar{h}_{ij}(t, r) = \begin{pmatrix} h_+ & h_\times & 0 \\ h_\times & -h_+ & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

where h_+ and h_\times are the gravitational wave polarizations, determine the expression for the gravitational wave strain $h(t, r) = h_+(t, r) + ih_\times(t, r)$, and, from it, provide the expressions for the strain amplitude h_0 and the wave angular frequency Ω . Substitute in the latter expressions the value of ω obtained in question 2. To get an idea of the orders of magnitude involved, provide the numerical value for both h_0 and Ω in the case of a binary black hole with $m_1 = m_2 = 30M_\odot$ separated a distance $R = 500$ km. Use $G = 6.7 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$, $M_\odot = 2 \times 10^{30} \text{ kg}$, and $c = 3 \times 10^8 \text{ m/s}$.

The gravitational strain polarizations are

$$\begin{aligned}h_+(t, r) &= -\frac{4G\mu R^2 \omega^2}{c^4 r} \cos 2\omega t_r, \\ h_\times(t, r) &= -\frac{4G\mu R^2 \omega^2}{c^4 r} \sin 2\omega t_r,\end{aligned}$$

so the gravitational strain is

$$h(t, r) = -\frac{4G\mu R^2 \omega^2}{c^4 r} [\cos 2\omega t_r + i \sin 2\omega t_r] = \frac{4G\mu R^2 \omega^2}{c^4 r} e^{i(2\omega t_r + \pi)},$$

from which

$$\begin{aligned}h_0 &= \frac{4G\mu R^2 \omega^2}{c^4}, \\ \Omega &= 2\omega.\end{aligned}$$

Substituting into these two expressions the value found in question 2 for ω , we finally obtain

$$\begin{aligned}h_0 &= \frac{4G\mu R^2 \omega^2}{c^4} = \frac{4G^2 M \mu}{c^4 R} = \frac{4G^2 m_1 m_2}{c^4 R}, \\ \Omega &= 2\sqrt{\frac{GM}{R^3}}.\end{aligned}$$

Substituting the numerical values provided, we find:

$$h_0 = \frac{4 \times (6.7 \times 10^{-11})^2 \times (6 \times 10^{31})^2 \text{ m}^6 \text{ kg}^{-2} \text{ s}^{-4} \text{ kg}^2}{(5 \times 10^5) \times (3 \times 10^8)^4 \text{ m}^5 \text{ s}^{-4}} = 1.5 \times 10^4 \text{ m},$$

$$\Omega = 2 \sqrt{\frac{(6.7 \times 10^{-11}) \times (1.2 \times 10^{32}) \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2} \text{ kg}}{(5 \times 10^5)^3 \text{ m}^3}} = 2 \times 0.25 \times 10^3 \text{ s}^{-1} = 500 \text{ s}^{-1}.$$

5. **(1 point)** Determine whether, for the frequency Ω corresponding to the example of binary system considered in question 4, the LIGO interferometers (see Fig. 7) are sensitive enough to the signals they emit.

In our situation, $f = \Omega/2\pi \approx 79.58 \approx 80$ Hz. The curves around this frequency in Fig. 3 are lower about 10^{-46} , which gives a maximum amplitude of at least $10^{-23} < 10^{-21}$. So, the interferometers are sensitive enough to the signals requested.

6. **(1 point)** Assuming that the detection threshold is $|h| \gtrsim 10^{-21}$, how far away can the system be for it to still be detected? Express the distance in multiples of a parsec ($1 \text{ pc} = 3.1 \times 10^{16} \text{ m}$).

$$10^{-21} \lesssim |h| = \frac{h_0}{r} \Rightarrow r_{\max} = \frac{h_0}{10^{-21}} = \frac{1.5 \times 10^4 \text{ m}}{10^{-21}} \frac{1 \text{ pc}}{3.1 \times 10^{16} \text{ m}} = 4.8 \times 10^8 \text{ pc} = 480 \text{ Mpc}.$$

7. **(1.5 points)** Estimate the rate of binary black hole mergers in the universe taking into account that the first three rounds of observation of the LIGO Interferometers have had a combined duration of 448 days, and, in this time, 90 signals have been successfully identified. Express the rate in mergers/Gpc³·yr.

We will detect any merger that occurs at a distance $d \lesssim 480$ Mpc. This space encapsulates a sphere of volume

$$V = \frac{4}{3}\pi R^3 = 0.46 \text{ Gpc}^3.$$

The rate of mergers is then

$$R = \frac{90 \text{ mergers}}{448 \text{ days}} \frac{1}{0.46 \text{ Gpc}^3} \frac{365 \text{ days}}{1 \text{ year}} \approx 150 \text{ mergers/Gpc}^3 \cdot \text{yr}.$$