

MATHEMATICAL MODELING FOR PHYSICAL SCIENCES

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ABSTRACT. Abstract goes here :)

1. GUIDE

This section provides with guidelines to approach the mathematical modeling of physical phenomena.

1.1. Problem background. A mathematical model of a physical phenomenon begins with the *problem background*, a description or introduction to the object. It should contain

- a *description* of the essential features of the physical process and
- an identification of the *objectives*, the key questions requiring answers.

Answering what, who, where, how and why questions guides to write down the description. Additionally, including graphical illustrations aids not only in the description, but in the definition of physical quantities and the establishment of hypotheses, as well.

1.2. Problem formulation. The *problem formulation* aims to:

- identify key physical processes;
- interpret these processes mathematically;
- establish a mathematical model – governing equations and suitable initial and boundary conditions;
- state clearly the assumptions.

The formulation must be based on sound physical principles, experimental facts or laws expressed in mathematical terms. As a guide, then, define the physical framework (geometry, kinematics, dynamics, thermal transfer and so on), state a dimensional set and then define the physical quantities, constants, parameters, coefficients and provide their dimensions in the chosen set.

A more formal approach is to begin with educated guessing, followed by dimensional analysis, order of magnitude analysis¹, analysis of extreme cases, simplifications and ends with a restricted model. The end result may be less accurate to fit experimental data, but less complex and thus more understandable. If fitting is not satisfactory, one can relax simplifications, one at a time, until a desired, or required, agreement is found.

1.3. Analysis. Once the physical and mathematical models and their assumptions have been proposed, one regularly faces a set of equations, probably differential equations together with initial and boundary conditions. The next step is then to analyze the set by

- non-dimensionalize the equations, included initial and boundary conditions;
- making analogies with other related problems or phenomena, as the case of mass, energy and momentum transport and
- relying on analytic and numeric methods, obtaining solutions (results).

In the case of obtaining analytic solutions to differential equations, it is necessary to verify that they satisfy the differential equations object to the initial and boundary conditions.

As a final step, uncertainty analysis should be performed, to obtained ranges of validity, instead of punctual solutions.

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Key words and phrases. mathematical modeling.

¹Order of magnitude analysis is preceded by dimensional analysis, since *only* the comparison of *dimensionless* quantities is meaningful!

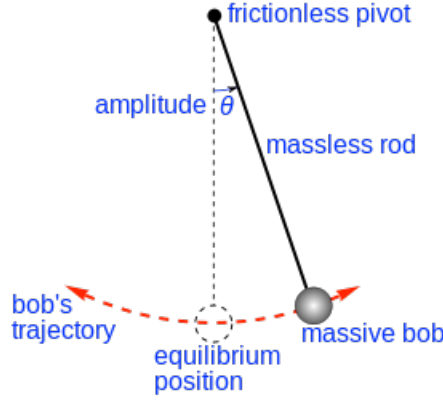


FIGURE 1. Schema of a simple gravitational pendulum

1.4. **Results.** The final step of modeling physical phenomena is to present results, give conclusions and discussion them. Specifically, one should

- interpret results with respect to the original physical process and objectives;
- verify assumptions by confronting the results with reference values or experimental data and
- identify the solution limitations and possible extensions.

2. BACKGROUND

In this section, we set the description of a physical phenomenon: the motion of a gravitational pendulum. We focus on answer the questions: what is a pendulum? what is a gravitational pendulum? How the pendulum is set into motion? What keeps the pendulum moving? What forces act on the pendulum that damp its motion? We also provide a bit of some historical information about it.

2.1. **Description.** A *pendulum* is a mechanical system consisting of a bob hanging by a rod attached to a pivot. A *gravitational pendulum* is a pendulum object only to gravitational interactions. Finally, a *simple gravitational pendulum* is a gravitational pendulum consisting of a massive bob hanging by a massless rod attached to a frictionless pivot. Figure 1 depicts a simple pendulum.

For all the pendulums, at any time t , the angle made by the rod with respect to the vertical, the pendulum equilibrium position, is called the *pendulum amplitude*, θ . The *pendulum trajectory*, $\theta[t]$, is found by joining the different θ at their corresponding t . Lastly, the *pendulum angular velocity*, $\dot{\theta}$, can be calculated as the time derivative of θ .

Returning to the physical description, a gravitational pendulum is set into motion by:

- (1) moving the bob from its equilibrium position to an initial amplitude, θ_0 , at an initial time;
- (2) applying a force that imprints an angular velocity to the bob at an initial time, $\dot{\theta}_0$, or
- (3) both at the same initial time.

Once motion starts, the system acquires *kinetic energy*, e_{kin} , that is then balanced by *gravitational potential energy*, e_{pot} . This restoring energy causes the system to oscillate about the equilibrium position, swinging back and forth. The time for one complete cycle, a left swing and a right swing, is called the *pendulum period*, τ . The interplay between both energies continues indefinitely, unless an external force, such as a *damping force*, stops the pendulum from moving. Friction at the pivot or fluid drag, provided a partial or total pendulum submersion in a viscous fluid, are examples of damping forces. Finally, buoyancy is another force that comes into play by effectively reducing the bob weight.

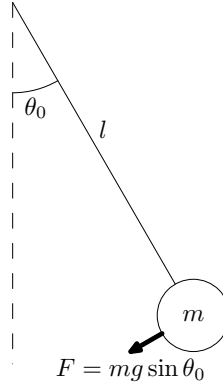


FIGURE 2. A pendulum bob of mass m hangs from a massless rope of length l . The bob is released from rest at an angle θ_0 .

A bit of history. Galileo Galilei studied pendulums *ca.* 1600. He discovered that the pendulum periods are *isochronos*; *i.e.*, the period is independent of the initial amplitude. Then, by further studies, Christiaan Huygens proposed that the pendulum period depends on the square of its length. More precisely:

$$\tau = 2\pi\sqrt{\frac{l}{g}}, \quad (1)$$

where l is the rod length and g the free fall acceleration. This equation is known as *Huygens' law for the period*. See, finally, that Huygens' law is consistent with the Galilei's isochronos result.

2.2. Objective. The aim herein is to find a closed form of a mathematical function to predict the trajectory of a gravitational pendulum. A closed form may perhaps not be found when modeling a real gravitational pendulum, thus restrictions based on sound physical arguments would need be made.

3. PHYSICAL PROCESSES

There are two main classes of gravitational pendulum motion: *undamped motion* – no frictional forces nor drag considered – and *damped motion* – friction and drag acknowledged. In both cases, however, the interplay between the pendulum kinetic energy and gravitational potential need be accounted, since it drives motion.

To begin with, we estimate the period of a simple gravitational pendulum by using educated guessing. This stage will sketch and, hopefully backup, more formal theoretical and mathematical analysis of the system.

Next, to uncover the relationships among the physical quantities that may affect the pendulum motion, we firstly propose formally such quantities, join then them as dimensionless quantities and use finally physical arguments to restrain the physical model. The last step will pave the path to a simple, however accurate, mathematical model.

3.1. Educated guessing. Before performing lengthy theoretical calculations, we use simple physical considerations to estimate some pendulum quantities. In concrete, we present an assessment for the the pendulum period by approximating the pendulum tangencial acceleration and the oscillation distance. We apply Newtonian mechanics arguments to the case of a simple gravitational pendulum.

[Figure 2 source: Sanjoy Mahajan, Order of Magnitude Physics A Textbook with Applications to the Retinal Rod and to the Density of Prime Numbers. PhD Thesis. California Institute of Technology Pasadena, California. 1998]

Consider fig. 2. The pendulum bob is object of a force $\sim mg \sin[\theta_0]$ that accelerates it at $a \sim g \sin[\theta_0]$. For small θ_0 , then $a \sim g\theta_0$. In time τ , the bob moves a distance

Quantity	Symbol	Dimension
bob amplitude	θ	1
bob initial amplitude	θ_0	1
bob mass	m_{bob}	M
bob density	ρ_{bob}	M/L ³
bob diameter	d_{bob}	L
rod length	l_{rod}	L
rod mass	m_{rod}	M
torque at pivot	τ	ML ² /T
pivot friction coefficient	α	1
fluid density	ρ_{fl}	ML ³
fluid dynamic viscosity	μ	M/LT
time	t	T
free fall acceleration	g	L/T ²

TABLE 1. Physical quantities involved in the motion of a gravitational pendulum

$a\tau^2 \sim g\theta_0\tau^2$. On the other hand, to complete a cycle, it needs to travel a distance $\lambda \sim l\theta_0$, so $g\theta_0\tau^2 \sim l\theta_0$. With that, the estimation of τ is

$$\tau \sim \sqrt{l/g}.$$

This result is consistent with Huygens's law, eq. (1), and Galilei's isochronous observation.

Alternatively, as a cross-check calculation, we can estimate a typical bob velocity and with it approximate the period. The maximum potential energy is $e_{\text{pot}} \sim mgh$, where ² $h = l(1 - \cos[\theta_0]) \sim l\theta_0^2$. The maximum kinetic energy equals the maximum potential energy, since a simple pendulum is undamped. The maximum velocity can be found by $mv^2 \sim mgl\theta_0^2$, which yields $v \sim \theta_0\sqrt{gl}$, an estimate for a typical velocity. The period is finally $\tau \sim \lambda/v \sim \sqrt{l/g}$, as found using force and acceleration.

3.2. Dimensional and order of magnitude analyses. In this section, we show how to use dimensional and order of magnitude analyses to reduce modeling complexity. We do this by considering first damped pendulum motion and then by going gradually to undamped motion by means of physical reasoning.

3.2.1. Dimensional analysis. Since the problem belongs to dynamics, choose the dimensional set $\{\text{L}, \text{M}, \text{T}\}$, with a cardinality of three. Next, as in table 1, list the possible physical quantities that may influence the pendulum motion along with their symbols and dimensions ³ in the chosen set.

A first approach may be to model the pendulum amplitude by a function f of the form

$$\theta = f[\theta_0, t, g, l_{\text{rod}}, m_{\text{rod}}, \tau, \alpha, m_{\text{bob}}, \rho_{\text{bob}}, d_{\text{bob}}, \rho_{\text{fl}}, \mu].$$

This complex relationship can be organized by means of dimensional analysis.

To begin with, since ρ_{bob} , m_{bob} and d_{bob} are related, discard mass. With this reduction, there are 12 physical quantities and 3 independent dimensions. Thus, according to the Pi-theorem, $12 - 3 = 9$ dimensionless quantities, $\{\Pi_i\}$, can be formed. Choose these dimensionless quantities as

$$\begin{aligned} \Pi_1 &= \theta, \Pi_2 = \theta_0, \Pi_3 = t\sqrt{\frac{g}{l}}, \\ \Pi_4 &= \alpha, \Pi_5 = \frac{m_{\text{rod}}}{m_{\text{bob}}}, \Pi_6 = \frac{(m_{\text{bob}} + m_{\text{rod}})gl_{\text{rod}}}{\tau}, \\ \Pi_7 &= \frac{d}{l}, \Pi_8 = \frac{\rho_{\text{fl}}}{\rho_{\text{bob}}}, \Pi_9 = \frac{\rho_{\text{fl}}d\sqrt{lg}}{\mu}. \end{aligned}$$

² The first term of the Taylor series for $(1 - \cos[\theta])$ is $\theta^2/2$. The incurred error is of order θ^4 .

³ The model for the friction at the pivot is $\tau = \alpha mgr$, where α is the friction coefficient, m the mass supported by the pivot and r the radius of the axis or rod supporting the pivot.

See that Π_1 contains the quantity being sought, θ , that Π_2 the quantity that originates motion, θ_0 , and Π_3 the (independent) quantity against which to confront motion, t . Now, again using the Pi-theorem, the desired *dimensionless* function, ϕ_π , has the *form*:

$$\theta = \phi_\pi \left[\theta, \theta_0, t \sqrt{\frac{g}{l}}, \alpha, \frac{m_{\text{rod}}}{m_{\text{bob}}}, \frac{(m_{\text{bob}} + m_{\text{rod}}) g l_{\text{rod}}}{\tau}, \frac{d}{l}, \frac{\rho_{\text{fl}}}{\rho_{\text{bob}}}, \frac{\rho_{\text{fl}} d \sqrt{lg}}{\mu} \right]. \quad (2)$$

To reduce the complexity of the mathematical model, restrain the physical model by working on the pendulum, by doing order of magnitude analysis and by making assumptions. Under such hypotheses, we will go from a damped motion case to an undamped motion case.

3.2.2. Order of magnitude analysis. First, consider a *frictionless pivot*. Proper lubrication of the pivot reduces friction. With this, the frictional torque term disappears. To support this assumption, consider that a dry and clean joint of steel pivot and steel rod has a friction coefficient of 0.80, while when lubricated 0.16.

Next, consider a *massless, inflexible rod*. The rod may be build of a strong material; strong enough to support the bob without elongating. This allows the construction of a very thin rod, with which the ratio of masses vanishes.

Use now order of magnitude analysis to further restrain the model. Consider a rod length much greater than the bob length. This is possible since we build the pendulum with a very strong rod. Say, for instance, that the bob diameter is 5 cm and the rod length 1 m, then $d/l = 0.05$, which can be neglected.

Consider an non-buoyant fluid by encasing the pendulum and surrounding it by air. The bob density will then be greater than air density. For example, if the system is at 15 °C, at sea level, and the bob made of steel, then

$$\frac{\rho_{\text{air}}}{\rho_{\text{steel}}} = \frac{1.225 \text{ kg/m}^3}{7750 \text{ kg/m}^3} \sim 0.158 \times 10^{-4},$$

which can be ignored.

Consider air as an *inviscid fluid*. An inviscid fluid is a fluid with no viscosity, resulting thus in no drag. To back up this assumption, plug some typical values into Π_9 :

$$\frac{\rho_{\text{air}} d_{\text{bob}} \sqrt{lg}}{\mu} = \frac{1.225 \times 0.05 \sqrt{1.00 \times 9.80665}}{1.983 \times 10^{-5}} \sim 9672,$$

where values in SI units were used. See that inertial forces, $\rho_{\text{air}} d_{\text{bob}} \sqrt{lg}$, are larger than viscous forces, μ . Thus, discard viscosity.

Finally, after having restrained the physical model, we seek for a mathematical function of the form

$$\theta = \phi_\pi \left[\theta_0, t \sqrt{\frac{g}{l}} \right]. \quad (3)$$

Neither dimensional analysis nor order of magnitude analysis can help to find the functional form of ϕ_π . It must be found by a more refined theoretical analysis or by experimentation. Nevertheless, based on sensible assumptions, we have reduced the complex physical model by passing from 13 dimensional quantities to 3 dimensionless quantities. At the end of the day, however, only confrontation with experimental data will support or disprove the reductions we have done.

3.2.3. Further implications. Considering an undamped system implies that mechanical energy *must* be conserved, for only kinetic energy turns into gravitational potential energy and *vice versa*. Hence, use Lagrange's and Hamilton's formulations of mechanics, instead of Newton's, to analyze the system.

Incidentally, eq. (3) may seem, at first sight, a very restricted model. It is, nevertheless, a practical one: a longcase clock pendulum. Such a clock consists of case full of air holding inside a heavy bob hanging by a light and inflexible rod attached to a lubricated pivot.

3.3. Mathematical interpretation. For the gravitational pendulum, we begun seeking a mathematical relationship of the form presented in eq. (2). Then, after sensible physical considerations were made, we ended with a restricted model of the form eq. (3).

The physical assumptions that we made in eq. (2) translate mathematically into

- A frictionless pivot implies no torque. Thus, $\Pi_4 = \Pi_6 = 0$.
- A massive bob hanging of a massless and inflexible rod implies that $\Pi_5 = 0$.
- A bob diameter much smaller than rod length results in $\Pi_7 = 0$.
- A bob made of steel swinging through air, air being less dense than steel, gives a non-buoyant fluid. Thus, $\Pi_8 = 0$.
- Air considered as inviscid, implies no viscosity, thus no drag. Therefore, $\Pi_9 = 0$.

Finally, for the sake of mathematical purposes, we can combine all the previous assumptions by defining a *simple gravitational pendulum*:

a simple gravitational pendulum is a pendulum composed of a massive bob hanging by a massless and inflexible rod attached to a frictionless pivot. Under the influence of gravitational interactions, the pendulum swings through an inviscid fluid of negligible density.

3.4. Mathematical model. In this section, we deduce the equation of motion for a simple gravitational pendulum by means of Lagrange's formulation mechanics by assuming that the pendulum is set into motion by displacing the bob an initial angle θ_0 with no further forces, $\dot{\theta}_0 = 0$.

Consider a simple gravitational pendulum composed of a bob of mass m and a rod of length l . Let θ be the amplitude of the pendulum for any time t , the initial angle be θ_0 , the initial velocity be $\dot{\theta}_0 = 0$ and, finally, g be the free fall acceleration. Then, find the equation of motion for the pendulum.

Using θ as the generalized position and $\dot{\theta}$ as the generalized velocity, write down the Lagrangian, e_{lag} , for the system:

$$e_{\text{lag}} = \frac{1}{2}ml^2\dot{\theta}^2 - mgl(1 - \cos[\theta]) . \quad (4)$$

Find next the generalized momentum, p_θ , and its temporal change, \dot{p}_θ :

$$p_\theta = \partial_{\dot{\theta}}e_{\text{lag}} = ml^2\dot{\theta} \implies \dot{p}_\theta = d_t\partial_{\dot{\theta}}e_{\text{lag}} = ml^2\ddot{\theta} . \quad (5)$$

Calculate then the generalized force, f_θ :

$$f_\theta = \partial_\theta e_{\text{lag}} = -mgl \sin[\theta] .$$

Replace the generalized force and the temporal change of the generalized momentum in Euler-Lagrange's equation:

$$f_\theta = \dot{p}_\theta \implies ml^2\ddot{\theta} + mgl \sin[\theta] = 0 .$$

Since $ml > 0$, divide the last equation through ml^2 to have

$$\ddot{\theta} + \frac{g}{l} \sin[\theta] = 0 .$$

Finally, rewrite the last equation by joining to it the initial conditions

$$\begin{cases} \ddot{\theta}[t] + \frac{g}{l} \sin[\theta[t]] = 0 , \\ \theta[0] = \theta_0 , \\ \dot{\theta}[0] = 0 , \end{cases} \quad (6)$$

which yields the equation of motion for a simple gravitational pendulum.

3.5. Assumptions. The equation of motion for the pendulum was found using the assumptions made in section 3.2 and summarized in section 3.3.

4. ANALYSIS

In this section, we solve the mathematical model of the simple gravitational pendulum, eq. (6).

4.1. Non-dimensional analysis. The independent quantity is t , the dependent quantity θ and the parameters are θ_0 , l and g . Since θ is already dimensionless, non-dimensionalize t to \bar{t} by using Π_3 as scaling factor:

$$\bar{t} = \Pi_3 = t\sqrt{\frac{g}{l}} \implies t = \bar{t}\sqrt{\frac{l}{g}}.$$

Find next the \bar{t} differentials

$$dt = d\bar{t}\sqrt{\frac{l}{g}} \implies dt^2 = d\bar{t}^2 \frac{l}{g}.$$

Replacing the last expressions in eq. (6) and dividing the result through $g/l(> 0)$, find the dimensionless and parameter-free differential equation:

$$\begin{cases} \ddot{\theta} + \sin[\theta] = 0, \\ \theta[0] = \theta_0, \\ \dot{\theta}[0] = 0, \end{cases} \quad (7)$$

where the derivatives are to be taken with respect to \bar{t} .

4.2. Analytic solution. Equation (7) is a non-linear, second-order ordinary differential equation. Linearize it by means of the *small-angle approximation*⁴:

$$\begin{cases} \ddot{\theta} + \theta = 0, \\ \theta[0] = \theta_0, \\ \dot{\theta}[0] = 0. \end{cases}$$

The solution to this equation is

$$\theta[\bar{t}] = \theta_0 \cos[\bar{t}], \quad (8)$$

or, returning to the dimensional quantity t ,

$$\theta[t] = \theta_0 \cos\left[t\sqrt{\frac{g}{l}}\right], \quad (9)$$

which solves eq. (6) for $\theta \ll 1$.

5. RESULTS

Although physically and mathematically restrained with respect to the original problem, an undamped pendulum, eq. (9) does provide a closed form function to predict the amplitude variation of a simple gravitational pendulum with respect to time.

Hereafter, we discuss this equation under physical grounds – conservation laws – and confront its predictions with experimental data.

5.1. Theoretical discussion. In this section, we investigate whether eq. (9) satisfies the principles of momentum and energy conservation.

[consistency on the description of motion: when particle moves to the right, the force points to the left (grav. potential energy restores kinetic energy), and *vice versa*.

circular motion: amplitude describes a circle, since inflexible rod]

⁴ The *small-angle approximation* means to take the first term of the Taylor series for $\sin[\theta]$ when $\theta \ll 1$; i.e., $\sin[\theta] \sim \theta$ for $\theta \ll 1$. The incurred error is of order θ^3 .

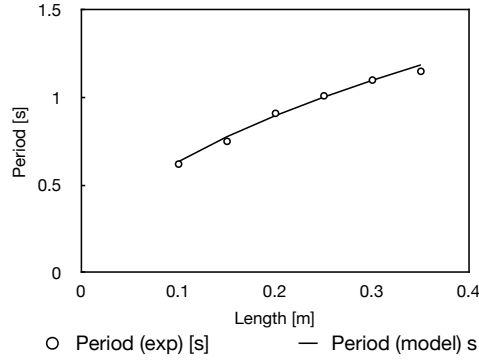


FIGURE 3. Model values for the simple gravitational pendulum and experimental data gathered from a real gravitational pendulum

5.1.1. *Momentum conservation.* Momentum of a system is conserved if there are no interactions; *i.e.*, $dp = 0$. Now, since we departed from the hypothesis that gravity acts on the simple gravitational pendulum, eq. (9) should *not* preserve momentum⁵.

To begin with, find the pendulum angular velocity by differentiating eq. (8), the dimensionless form of eq. (9), with respect to \bar{t} :

$$\dot{\theta} = d_{\bar{t}}\theta = -\theta_0 \sin[\bar{t}] . \quad (10)$$

Next, replace the pendulum angular velocity in eq. (5), the pendulum momentum:

$$p_{\theta} = ml^2\dot{\theta} = -ml^2\theta_0 \sin[\bar{t}] .$$

Finally, find the momentum time derivative:

$$\dot{p}_{\theta} = -ml^2\theta_0 \cos[\bar{t}] .$$

Since \dot{p}_{θ} is *not* zero, momentum is *not* conserved during motion. Thus, eq. (9) accords with physical principles.

5.1.2. *Energy conservation.* In Hamilton's formulation of mechanics, the Hamiltonian of a system equals the system total energy. Thus, if the total energy is conserved, then the Hamiltonian time derivative must be null. In the case of the simple pendulum, eq. (9) *should* conserve total energy, since we hypothesized an undamped system.

Firstly, write down the Hamiltonian, e_{ham} , of the system:

$$e_{\text{ham}} = e_{\text{kin}} + e_{\text{pot}} = \frac{1}{2}ml^2\dot{\theta}^2 + mgl(1 - \cos[\theta]) .$$

Replace $(1 - \cos[\theta])$ by the first term of its Taylor series:

$$2e_{\text{ham}} = ml^2\dot{\theta}^2 + mgl\theta^2 .$$

Plug eq. (8) and eq. (10) into the last equation to have

$$2e_{\text{ham}} = ml\theta_0^2 (l \sin^2[\bar{t}] + g \cos^2[\bar{t}]) .$$

Finally, derivate the last equation with respect to \bar{t} :

$$d_{\bar{t}}e_{\text{ham}} = ml\theta_0^2 (l \sin[\bar{t}] \cos[\bar{t}] - g \sin[\bar{t}] \cos[\bar{t}]) .$$

Since $d_{\bar{t}}e_{\text{ham}}$ does *not* equal zero, eq. (9) does *not* satisfy the energy conservation principle. This discrepancy originates due to the small-angle approximation.

5.2. Experimental data and reference values. Experimental data was not specifically gathered for writing the present document. However, some reference values were found in the internet [source!]. Such values together with the model predictions of eq. (9) are presented in fig. 3.

Using fig. 3, one finds that the *coefficient of determination*, R^2 , between model figures and experimental data is 0.9876, while the relative error 2.03 %. Both figures show agreement between model and experiment, thus eq. (9) is taken to correctly represent real pendula.

Nevertheless, if more accuracy is required or less agreement is found when applying eq. (9) to a real pendulum, then the model can be extended by relaxing the assumptions made in section 3.5. For instance, if the pendulum swings through a viscous fluid, such as a liquid, then the dimensionless quantities Π_8 and Π_9 should be included. Or, if there is little care in lubricating the pivot, then Π_4 , Π_5 and Π_6 should be further studied.

5.3. Analogies with other phenomena. In classical *simple harmonic motion*, the period of the motion, τ , is the time required for a complete oscillation and defined by

$$\tau = \frac{2\pi}{\omega},$$

where ω is the motion *natural frequency*.

The motion of a simple gravitational pendulum, described by eq. (9), is an instance of simple harmonic motion, where θ_0 is the semi-amplitude of the oscillation and where the natural frequency is

$$\omega = \sqrt{\frac{g}{l}}.$$

The period of the pendulum motion, for the outward and return, is thus

$$\tau = 2\pi\sqrt{\frac{l}{g}}. \quad (11)$$

The last equation is Christiaan Huygens's law for the period.

Note that only under the small-angle approximation, the period is independent of the amplitude θ_0 ; *i.e.*, *isochronism* – the property Galileo discovered.

⁵ In the grand scheme of things, momentum *is* conserved, but to see this, we would need to add Earth's momentum as well as the pendulum's.