Lecture notes

The Physics Compendium

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Introduction

This book serves a dual purpose - one is to record my understanding and knowledge about the topic, and related to it, and one is to develop my own theories and models - most likely original, more often than not it's not. Also, it will also include rough implementation, papers' ideas analysis, and else. So, a bag full of everything, I suppose. a dual purpose - one is to record my understanding and knowledge about the topic, and related to it, and one to directly record and write down my discovery, or rather, most of the time just analysis and designs.

It might sound as if this book is entirely self-sufficient, and also self-serving, yet it isn't. The text cannot take into account all preliminaries or requirements of understanding, yet. It is simply too large to take all in, because the field itself is very complex. Self-serving side, perhaps it can be broken down to 0-1 loss function two (it's a joke), since it is perhaps too difficult to follow directly from the get-go, so I pretend to be the third-party narrative. With that, the book is not just about myself asking and answering questions, logging knowledge, but to also write and try to explain it as a perhaps to a 5-year-old, to somehow make it sounds not like listening to quantum mechanics.

Overall, I seriously hope that this book will help me myself, ultimately, and help anyone along the way, if they stumble upon this. Hopefully you will give me some exposure too (famous?), so, I am counting on you. With that said, artificial intelligence is a hoax. Only us can refute that.

What is in the book

The book is concerned of the main umbrella topic of artificial intelligences. Alongside with it are relevant theories and practical implementations that support said theoretical view. So, you would also expect to have *machine learning*, *mathematical modelling*, *a lot of mathematics*, *information theory*, *complexity analysis*, and more. Specifically, there will also be an entire large chapter on the formalism of the learning theory, in a rigorous sense, so many of the chapters would be there to reinforce this.

As it currently stands, the main top category is the parts. Specifically, there are three main parts. Part I on *theory* – the supporting theory, discussions, results and analysis. Part II on *advanced theory*, being called advanced just because it is my own implementation and theory in accordance. And part III on *implementation* and any necessary details on such – so, it can contain sections on the Python language itself (which is boring) – but also sections concerning deployment or rather typical construction of what has been established in the preceding part. Though there are plans to go for C++ implementation, high-intensity computation is perhaps not in the list for the current time (April 2024).

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How much topic is covered?

Well, not so much, but I hope it will be enough to formalize and construct a formal treatment of a potentially modern approach to artificial intelligence theory. Of the latest revision, however (May 18, 2025), the book has been subsequently changed of its status as a comprehensive AI-based book, to a rather general book by its own standard. Though, it does not contrive the structure for literally everything, so mostly we will narrow down to either philosophy, computer science theory, artificial intelligence, mathematics, and physics.

I. Physics

The physical world where all things reside, where all phenomena are observed, and of all life and purposes, to be given meaning.

Edmund. D. K.

Chapter 1. Electromagnetism

This chapter is dedicated entirely to electromagnetism, the theory of moving charge. So, even though this section of introduction might seem a bit short, I think it is enough. Probably.

1.1 Electrostatic

We introduce a few "introductory" concepts, which we call the theory of stationary charge, electrostatic. The more application-al, circuit implementation was reserved for the general physics chapter, so we would not touch on such subject.

1.1.1 Electric charge

The basic, and the most fundamental quantity that gave rises to the field of electrodynamics and the study of electricity, is *charge*. The two important aspects of charge are conservation and quantization, of which the electric force is as

$$E \sim \frac{1}{r^2}$$

with distance.

Classical electromagnetism deals with electric charges and currents and their interactions as if all the quantities involved could be measured independently, with unlimited precision. Here *classical* means simply nonquantum. The quantum law and \hbar is ignored here, just as in ordinary mechanics.

In this chapter, however, we shall focus on the physics of stationary electric charges - *electrostatics*.

Properties of electrical charges (1)

The first fundamental property of electric charge is its existence in the two varieties of **positive** and **negative**. This is an observed fact, that all charged particles can be divided into two classes, such that all members of one class repel each other, while attracting members of different class.

This is synonymous to the notion of symmetry, such that, for every kind of particle in nature, there can exist an *antiparticle*, of the mirror image, of which carries the charge of the opposite sign. If any other intrinsic quality of the particle has an opposite, the antiparticle has that too. In such case, the basic charge carrying particle electron has its counterpart being the **positron**. However, as we shall see, there are *abundant* of matters, rather than antimatters in the universe. The abundant carriers of negative charge are electron, while positive being protons, even though the mass comparability is around

$$m_e \approx \frac{1}{2000} m_p$$

so, usually, we view the positive charge in quite a distinct way.

Properties of electrical charges (2)

Two others properties of electric charge are essentially in the electrical structure of matter: charge is *conserved*, and *quantized*. These involve quantity of charges and thus imply a measurement of charge. Presently, we shall state precisely how charge can be measured in terms of the force between charges a certain distance apart and so on.

1.1.2 Conservation of charge

A quick review, we have the following conservation law: the **total charge** in an isolated system never changes.

Theorem 1.1.1 (Conservation law, first version). The total electric charge in an isolated system, that is, the algebraic sum of the positive and negative charge present at any time, never changes.

The creation of a positively charged particle hence **must** accompanied by the creation of a negatively charged particle. This is called as **pair-creation**.

1.1.3 Quantization of charge

The electric charge we find in nature come in units of one magnitude, equal to the amount of charge carried by a single electron, denoted as e. By sign, we either write it -e or (+)e respectively. Within empirical observations, we note also, that apparently, there is the exact equality of the charges carried by all other charged particles.

Specifically, proton and electron do not differ in magnitude of charge by more than 1 part in 10^{20} .

The equality that e=p is more likely of the theory that very rarely, proton will decay into a positron and some uncharged particles. If such event is to occur, it will show for certain, the equality being a corollary of the more general conservation laws. For now, well, there's none (too bad).

We know, however, that the internal structure of all the strongly interacting particles - hadrons including protons and neutrons, involve basic units called quarks, whose electric charges come in multiples of e/3. The proton is of the double

$$\left\{\frac{2e}{3}, -\frac{e}{3}\right\}$$

in terms of charge, while neutron is

$$\left\{\frac{2e}{3}, -\frac{e}{3}, -\frac{e}{3}\right\}$$

which makes it effectively no charge as expected.

However, it is only to that point that our conclusion drew out yet. We did not observe any stray fractional charge yet, and the present quantum theory of *quantum chromodynamic* tried to explain such as being impossible, too. The constitutions of the elementary particles are unknown, as it is for why the charge is fixed at certain value. But that is not too much of the concern for classical electromagnetism, as for now. Hence, we should treat the charged particle only as the *carriers of charges*.

1.1.4 Coulomb's law

The statement of the Coulomb's law is as followed.

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Definition 1.1.1 (Coulomb's law). Given two stationary electric charges q_1 and q_2 , Coulomb's law stated that they repel or attract one another with a force proportional to the product of the magnitude of the charges and inversely proportional to the square of the distance between them:

$$\mathbf{F}_2 = k \frac{q_1 q_2 \hat{r}_{21}}{r_{21}^2} \tag{1.1}$$

where \hat{r}_{21} is the unit vector in direction from $q_1 o q_2$, and ${f F}_2$ is the force acting from $q_1 o q_2$.

The unit vector $\hat{\mathbf{r}}_{21}$ shows that the force is parallel to the line joining the charge. This is not the case for the spin of the electron, which is very much smaller than the Coulomb's force, and the electrodynamic force when the electron moves (hence why the statement is about stationary particles).

We also assume that they are well localized, with a small region of occupation compared to r_{21} . The value of the constant k depends on the way that r, \mathbf{F} and q are expressed. For this, we use the SI system with q as Coulomb (C), and the unit k is expressed as:

$$k = 8.988 \cdot 10^9 \, \frac{Nm^2}{C^2} \tag{1.2}$$

for the following definition of Coulomb:

Definition 1.1.2 (Coulomb (unit)). Two like charges, each of 1 coulomb, would repel one another with a force of $8.998 \cdot 10^9$ Newtons when they are of unit meter distance.

Usually, instead of k it is customary to express it as

$$k = \frac{1}{4\pi\epsilon_0}$$

where

$$\epsilon_0 = \frac{1}{4\pi k} = 8.854 \cdot 10^{-12} \, \frac{C^2}{Nm^2}$$

The force is then expressed as:

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2 \hat{\mathbf{r}}_{21}}{r_{21}^2}$$

The 4π is the choice of simplicity in other quantities that use it.

One way to detect and measure electric charges is by observing the interaction of charged bodies. We have a following observation (after the three charges test):

Lemma 1.1.2. The force with which two charges interact is not changed by the presence of a third charge.

No matter *how many charges* we have in our system, Coulomb's law can be used to calculate the interaction of every pair. This is the basis of the principle of **superposition**, means combining two sets of sources into one system by adding the second system "on top of" the first without altering the configuration of either one. This ensures that the force on a charged placed at any point in the combined system will be the vector sim, of the forces that each set of sources acting alone causes to act on a charge at that point.

This principle must not however, taken lightly for granted. Indeed, there are cases in quantum electrodynamical phenomena that indicates the case where *superposition does not work*.

1.1.5 Energy of a system of charges

Energy is a useful concept in electrostatic, because electrical forces are **conservative**. Similar things happen in mechanics, however, we should see that there is a bit of a difference. Every action in charge movements are reversible, as there are no conceivable energy loss (But *why* so is not so much understood, I mean why? Why would there are no energy loss even if we apply certain amount of energy on it?). Consider moving two particles together. What is the work required to do such task?

It makes no difference if we bring q_1 or q_2 (the charges in question) in either way around, the work done is the integral of force and displacement, they being signed. The force that has to be applied to move one charge toward the other is equal and opposite to the Coulomb force:

$$W = -\int \mathbf{F} dr = \int_{-\infty}^{r_{12}} \left(-\frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r^2} \right) dr = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r_{12}}$$

The sign here is consistent. We are now setting up such that it is from 1 to 2, hence the direction of the applied force would be, negative, since they must be pushed together, hence the minus sign. The displacement is from infinity to r_{12} , hence also the minus sign being valid. This overall results in the positive work being done on the system. With q_1, q_2 in coulombs and r_{12} , they give the work in joules.

This work is the same whatever the path of approach, because the force is central (as we have expected) and radially outward. Returning to the charges, let us bring in some third charge q_3 and move it to a point P_3 whose distance from charge 1 is r_{31} , and r_{32} for q_2 , then

$$W_3 = -\int_{\infty}^{P_3} \mathbf{F}_3 d\mathbf{s} = -\int \mathbf{F}_{31} d\mathbf{s} - \int \mathbf{F}_{32} d\mathbf{s}$$

where s is the vectorized path. The total additive work is hence

$$U = \frac{1}{4\pi\epsilon_0} \left(\frac{q_1 q_2}{r_{12}} + \frac{q_2 q_3}{r_{23}} + \frac{q_1 q_3}{r_{13}} \right)$$

denoted U. One way of writing the instruction for the sum over pairs is this:

$$U = \frac{1}{2} \sum_{j=1}^{N} \sum_{k \neq j} \frac{1}{4\pi\epsilon_0} \frac{q_j q_k}{r_{jk}}$$

The double sum includes every pair twice, and to correct for that we put in front the factor 1/2.

1.1.6 Electric field

Suppose we have some arrangement q_1, \ldots, q_N fixed in space, and we are interested not in the forces they exert on one another, but only in their effect on some other charge q_0 that might be brought into their vicinity. The force on the charge q_0 in the coordinate field is

$$\mathbf{F} = \frac{1}{4\pi\epsilon_0} \sum_{j=1}^{N} \frac{q_0 q_j \hat{\mathbf{r}}_{0j}}{r_{0j}^2}$$

The force is proportional to q_0 so we can obtain a vector quantity that depends only on the structure of our original system of charge, and the position of the point (x, y, z) that the charge

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would occupy. We call this vector function of x, y, z the electric field arising from q_1, \ldots, q_N and use the symbol $\mathbf E$ for it. The charge q_1, \ldots, q_N we call sources of the field. The definition would be taken as for a charge distribution at the point (x, y, z):

$$\mathbf{E}(x, y, z) = \frac{1}{4\pi\epsilon_0} \sum_{j=1}^{N} \frac{q_j \hat{\mathbf{r}}_{0j}}{r_{0j}^2}$$

The force on other charge q at (x, y, z) is hence

$$\mathbf{F} = q\mathbf{E}$$

Unless the source charges are immovable, the electric field might shift because of the additional charge. The role of the electric field is quite useful:

- 1. It is another general interpretation.
- 2. It attaches to every point in a system a local property, without further inquiry, a charge's effective received influences in such neighbourhood.

In the neighbourhood of a true point charge, the electric field grows infinite like $1/r^2$ as we approach the point. It makes no sense to talk about the field <u>at</u> that point charge, as that will leave us to the mathematical singularity of infinite charge that would be subsequently ignored because charges are finite. So long as ρ remains finite, however, the field would remain finite everywhere, even in the interior or on the boundary of a charge distribution.

Chapter 2. Theoretical mechanics

2.1 Introduction

2.2 Calculus of variations

The *calculus of variations* involves finding the minimum or maximum of a quantity that is expressible as an integral. To see how this can arise, we have some examples.

2.2.1 The shortest path between two points

Given the two points in a plane, what is the shortest path between them? While the answer is a straight line, there are probably no proofs. Except if we can use calculus of variation. The problem is illustrated by two points, (x_1, y_1) and (x_2, y_2) , and a path, y = y(x) joining them. Our task is to find the path y(x) that has the shortest length and to show that it is in fact a straight line.

The length of a short segment of the path is $ds = \sqrt{dx^2 + dy^2}$, which, since

$$dy = \frac{dy}{dx}dx = y'(x)dx$$

we can rewrite it as

$$ds = \sqrt{1 + y'(x)^2} dx$$

Thus the total length of the path between points 1 and 2 is

$$L = \int_{1}^{2} ds = \int_{x_{1}}^{x_{2}} \sqrt{1 + y'(x)^{2}} dx$$

This equation puts our problem in mathematical form. The unknown problem now is the function y=y(x) for which the integral is the minimum, which, mind you, is not 0. It is interesting to contrast this with the standard minimization problem of elementary calculus, where the unknown is the value of x at which a known function f(x) is a minimum. Obviously, it is much more complicated than this old one. Before solving this problem, let's consider another example.

2.2.2 Fermat's Principle

A similar problem is to find the path that light will follow between two points. If the refractive index of the medium is constant, then the path is a straight line. But if it varies, or if we interpose a mirror or lens, the path is not so obvious. Fermat discovered that the required path is the path for which the time of travel of the light is minimum, v = c/n where n is the refractive index. Thus Fermat's principle says that the correct path between points 1 and 2 is

the path for which the time:

$$\sum t = \int_{1}^{2} dt = \int_{1}^{2} \frac{ds}{v} = \frac{1}{c} \int_{1}^{2} n \, ds$$

is a minimum. If n is constant, then it can be taken outside the integral and the problem reduces to finding the shortest path between points 1 and 2 (and the answer is, of course, a straight line). In general, the refractive index can very for n = n(x, y), and our problem is to find the path y(x) for which the integral

$$\int_{1}^{2} n(x,y) \, ds = \int_{x_{1}}^{x_{2}} n(x,y) \sqrt{1 + y'(x)^{2}} \, dx$$

is minimum.

The integral that has to be minimized in connection with Fermat's principle is very similar to the integral of the length of a path; it is just a little more complicated, since the factor n(x,y) introduces an extra dependence on x and y. Similar integrals arise in many other problems. Sometimes we want the path for which an integral is a maximum, and sometimes we are interested in both maxima and minima. It is helpful to think about this, as to give some ideas, to the problem of finding maxima and minima of functions in elementary calculus.

There, we know that the necessary condition for a maximum or minimum of a function f(x) is that its derivative vanish, dq/dx = 0. Unfortunately, this condition is not quite enough to guarantee a maximum or minimum. As you certainly recall from introductory calculus, there are essentially three possibilities, as illustrated in a typical introductory course in elementary calculus.

A point x_0 where df/dx is zero may be a maximum or a minimum, or if d^2f/dx^2 is also zero, it may be neither. When df/dx = 0 at a point x_0 but we don't know which of the three possibility obtains, we say that x_0 is a **stationary point** of the function f(x), since an infinitesimal displacement of x from x_0 leaves f(x) unchanged.

The method that is used to solve the shortest path problem, is actually to find the path that makes an integral like L to be stationary, in the sense that infinitesimal variation of the path from its correct course doesn't change the value of the integral concerned. If you need to know that the integral is definitely minimum, you have to check this separately. Since our concern is how infinitesimal variations of a path change an integral, the subject is, as we might have seen this, calculus of variations. For the same reason, the methods we shall develop are called of variational methods, and a principle like Fermat's is a variational principle.

calculus variations

2.2.3 The Euler-Lagrange equation

The two examples of the last section illustrate the general form of the so-called variational problem. We have an integral of the form

$$S = \int_{x_1}^{x_2} f[y(x), y'(x), x] dx$$

where y(x) is an as-yet unknown curve joining (x_1, y_1) and (x_2, y_2) , that is:

$$y(x_1) = y_1, \quad y(x_2) = y_2$$

Among all the possible curves satisfying 6.5, that is, joining points 1 and 2, we have to find the one that makes the integral S a minimum, or at least stationary. Though, as for what we want,

we wish for it to be a minimum. Because the integral follows the path y = y(x), the integrand is actually a function of just x.

Let us denote the correct solution to our problem by y = y(x). Then, the integral S in 6.4 evaluated for y = y(x) is less than for any neighbouring curve y = Y(x), as sketched in Fig 6.3. It is convenient to write the *wrong* curve Y(x) as

$$Y(x) = y(x) + \eta(x)$$

is the difference between the wrong Y(x) and the right y(x). Since Y(x) must pass through the endpoints 1 and 2, $\eta(x)$ must satisfy

$$\eta(x_1) = \eta(x_2) = 0 \quad (6.7)$$

There are infinitely many choices for the difference $\eta(x)$: for example, we could choose $\eta=(x-x_1)(x_2-x)$ or some form as $\eta(x)=\sin\left[\pi(x-x_1)/(x_2-x_1)\right]$. The integral S taken along the wrong curve Y(x) must be larger than that along the right curve, no matter how close the former is to the latter. To express this requirement, we shall introduce a parameter α and redefine Y(x) to be

$$Y(x) = y(x) + \alpha \eta(x)$$

The integral taken along the curve Y(x) now depends on the parameter α . We then call the integral for such as $S(\alpha)$. The right curve y(x) is obtained by $\alpha=0$. Thus the requirement that S is minimum implies that $S(\alpha)$ is minimum at $\alpha=0$. With this, we converted our problem from elementary calculus of making sure that an ordinary function has a minimum at a specified point. If we write out the integral $S(\alpha)$ in detail, it looks like:

$$S(\alpha) = \int_{x_1}^{x_2} f(Y, Y', x) \, dx = \int_{x_1}^{x_2} f(y + \alpha \eta, y' + \alpha \eta', x) \, dx$$

To differentiate this with respect to α , we note that α appears in the integrand f, so we need $\partial f/\partial \alpha$. Since α appears in two of the arguments of f, this gives two terms, namely:

$$\frac{\partial f(y+\alpha\eta,y'+\alpha\eta',x)}{\partial\alpha} = \frac{\eta(\partial f)}{\partial y} + \eta' \frac{\partial f}{\partial y'}$$

and for $dS/d\alpha$, which has to be zero, then

$$\frac{dS}{d\alpha} = \int_{x_1}^{x_2} \frac{\partial f}{\partial \alpha} dx = \int_{x_1}^{x_2} \left(\frac{\eta(\partial f)}{\partial y} + \eta' \frac{\partial f}{\partial y'} \right) dx = 0$$

This condition must be true for any $\eta(x)$ satisfying (6.7), that is, for any choice of the wrong path. We can rewrite the second term on the right using integration by parts, which gives us:

$$\int_{x_1}^{x_2} \eta'(x) \frac{\partial f}{\partial y'} dx = \left[\eta(x) \frac{\partial f}{\partial y'} \right] - \int_{x_1}^{x_2} \eta(x) \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) dx$$

Because of the condition in (6.7), the first term on the right is zero, hence we can remove them all. Thus,

$$\int_{x_1}^{x_2} \eta'(x) \frac{\partial f}{\partial y'} dx = -\int_{x_1}^{x_2} \eta(x) \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) dx$$

Substituting this into the equation above, we get

$$\int_{x_1}^{x_2} \eta(x) \left(\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} \right) dx = 0$$

This condition must be satisfied for any choice of the function $\eta(x)$. Therefore, the factor in the large parentheses must be zero, that is:

$$\frac{\partial f}{\partial y} - \frac{d}{dx} \frac{\partial f}{\partial y'} = 0$$

This is called the **Euler-Lagrange equation**, for all x in the interval $[x_1, x_2]$. This equation of Leonhard Euler and Joseph Lagrange lets us find the path for which the integral S is stationary. However, before that, we need to argue why we can say that the factor in the large parentheses must be zero.

Our above equation has the form

$$\int \eta(x)g(x)\,dx = 0\tag{2.1}$$

It would be not so nice to claim that this condition alone implies that g(x)=0 for all x. However, it needs to hold for all choice of $\eta(x)$, no matter how much it can be, and if the above integral is true for $\operatorname{any} \eta(x)$, then we can conclude that the only actionable factor here is that $g(x)=\alpha=0$. To prove this, we must assume that all functions concerned are continuous. Now, to prove this, let us assume the contrary that $g(x)\neq 0$ in some interval between x_1 and x_2 . Then, choose a function $\eta(x)$ that has the same sign as g(x), that is, positive when g(x) is, and negative when g(x) be. Then the integrand is continuous, satisfies $\eta(x)g(x)\geq 0$, and is non-zero in at least some interval. Under these conditions, the integral cannot be zero, which implies there exists no minimal path. This contradiction implies that g(x) is zero for all x. This completes the proof of the Euler-Lagrange equation.

2.2.4 More than two variables

So far we have considered only problems with just two variables, the independent variable (usually x) and the dependent (usually y). For most applications in mechanics, we shall find that there are several dependent variables, though through parameterization, there can be a singular independent variable, like t. For a simple example where there are two dependent variables, we can go back to the problem of the shortest path between two points. When we found the shortest path between two points 1 and 2, we assumed that the required path could be written in the form y = y(x). Reasonable as this seems, it is easy to think of paths that cannot be written in this way, such as this:

If we want to be perfectly sure we have found the shortest path among *all possible paths*, we must find a method that includes these. The way to do this is to write the path in parametric form as:

$$x = x(u)$$
 $y = y(u)$

where u is any convenient variable in terms of which the curve can be parameterized. The parametric form includes all the curves considered before. The length of a small segment of the path is then:

$$ds = \sqrt{dx^2 + dy^2} = \sqrt{x'(u)^2 + y'(u)^2} du$$

Thus, the total path length is:

$$L = \int_{u_1}^{u_2} \sqrt{x'(u)^2 + y'(u)^2} \, du$$

and our job is to find the two functions x(u) and y(u) that the integral is minimum. for now, the problem is more complicated than before, because there are now two unknown function

Euler-Lagrange equation x(u) and y(u). The general problem of this type is this: Given an integral of the form

$$S = \int_{u_1}^{u_2} f[x(u), y(u), x'(u), y'(u), u] du$$

between two fixed points $[x(u_1),y(u_1)]$ and $[x(u_2),y(u_2)]$, to find the path [x(u),y(u)] for which the integral S is stationary. The solution to this problem is very similar to the one-variable case, and we will perhaps analyse it for now. The upshot is that with two dependent variables, we get two Euler-Lagrange equations. To prove this, we proceed very much as before. Let the correct path given by

$$x = x(u)$$
 $y = y(u)$

and then consider a neighbouring "wrong" path of the form

$$x = x(u) + \alpha \xi(u)$$
 $y + y(u) + \beta \eta(u)$

The requirement that the integral S be stationary for the right path is equivalent to the requirement that the integral $S(\alpha, \beta)$ satisfies

$$\frac{\partial S}{\partial \alpha} = 0$$
 $\frac{\partial S}{\partial \beta} = 0$ $\alpha = \beta = 0$

The Euler-Lagrange is hence:

$$\frac{\partial f}{\partial x} = \frac{d}{du} \frac{\partial f}{\partial x'}$$
 $\frac{\partial f}{\partial y} = \frac{d}{du} \frac{\partial f}{\partial y'}$

A more generalized formulation will give you the notion of **generalized coordinates** and its configuration space.

2.2.5 Generalize formalism

The independent variable in Lagrangian mechanics is the *time t*. The dependent variables are coordinates that specify positions, or *configuration* of a system, denoted by q_1, \ldots, q_n . The number n of coordinates depends on the nature of the system. For a single particle moving unconstrained in three dimensions then n=3. Not that we say about unconstrained system, the 'free' configuration of the system in a constrained system is smaller, as well will see. The name generalized coordinates is inherently because, well, there are simply too many things about it that can specify the variables.

The goal of Lagrangian mechanics is to find how coordinates vary with time, or to find the n functions $q_1(t),\ldots,q_n(t)$. This is specified from Newton's law, yes, but also equivalent to the expression of Newton's law. Sometimes, it is even easier. The integral S whose stationary value determines the evolution of the system is called the <u>action integral</u>. Its integrand is called the <u>Lagrangian</u> \mathcal{L} and depends on the n coordinates, their derivatives, and t:

$$\mathcal{L} = \mathcal{L}(q_1, \dot{q_1}, \dots, q_n, \dot{q_n}, t)$$

Notice that since the independent variable is t, the derivative is denoted by the \dot{q} notation. The requirement for the integral S:

$$S = \int_{t_1}^{t_2} \mathcal{L}(q_1, \dot{q}_1, \dots, q_n, \dot{q}_n, t) \, dx$$

to be stationary implies n Euler-Lagrange equations:

$$\frac{\partial \mathcal{L}}{\partial q_1} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q_1}, \quad \dots \quad , \frac{\partial \mathcal{L}}{\partial q_n} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q_n}$$
 (2.2)

2.3 Lagrangian mechanics

The Lagrangian of classical mechanics depends on several notions. From the get-go, maybe this is realizable because we have been building up the calculus of variation technique. However, we are missing one final tool in the shed. So before that, we will have to find it.

2.3.1 Degree of freedom

The number of degrees of freedom determines how many generalized coordinates are in Lagrangian mechanics. Usually, the good way to calculate them is as followed. Note that even though the procedure looks easy, there are many times that you would have a hard time applying it. Also, there is this principle: If you cannot find the constraints, then give up and get the degree of freedom as it is.

Defining the dimension of the configuration space as the degrees of freedom, we then:

- 1. Determine the number of coordinate components (Cartesian, polar, spherical, etc.) for each component of the dynamical system (for example, the double pendulum is then the two masses). This is denoted by kN, where k is the component of the coordinate system, and N is the amount of objects.
- 2. Determine the constraint of the system, or the relational quantities for example, the length of the stick between the two pendulum. This is denoted by m.
- 3. Calculate the degrees of freedom the freely movable and dynamical part, as n = kN m.

By such, we can get a somewhat perfect representation of the degree of freedom of a system. This will ultimately justify the numbering of Lagrangian generalized coordinate, and this is also what and why we need the generalized coordinate consideration.

2.3.2 Lagrangian formalism

phase space

For a system, there exists its **phase space**, or the space of all possible configuration state that the system can be at a given time or incident. For example, the uniform circular motion will have the phase space as exactly the circle – as its evolution in time is subjected to position on the circle of radius r. By this, we can classify system based on how the phase space varies with time. If the phase space stays the same throughout its evolution in time, then we say the system is **conservative**. Else, if the system's phase space varies with time, then we call it **nonconservative**; in more detailed terms, we have **dissipative system** for system with reduced phase space, and **expanding system** for system with its phase space increased.

dissipative system expanding system

Newtonian mechanics is fully sufficient practically for interpreting and analysing mechanical system and behaviours. Indeed, sometimes with all the laws and $\vec{F}=m\vec{a}$, it is enough to specifies all the evolution and factors of the system. However, with increasingly complex system, Newtonian formalism becomes much more difficult to work on, as its basis of specifying forces and additives of system's components together. Instead, it is desirable to find a way to obtain equations of motion from some scalar generating function, or rather, some inherent qualities that encode information about the system into itself, and can be used to defer to the equation of motion, which is, of importance is the evolutionary law of any given system based on mechanics. For conservative systems, the complete information about the system is contained in the total energy:

$$E = E_k + U$$

This is expressed by a function of coordinates and velocities, or angles and their time derivatives for some system considered above. However, using this, there is no way to obtain equations of motion from the energy function directly. This can be deferred to the loss of information in the

reversing direction, for the given mathematical realization of the physical system backward. It turns out, however, that the generating function of equations of motion is the quantity called the Lagrangian (or Lagrange function), taken in the form

$$\mathcal{L} = E_k - U = T - U$$

The Lagrange formalism is build upon the so-called Least-Action principle, also called the Hamiltonian principle. According to this principle, that can be put into the foundation of mechanics, the actual dynamics of the system, that is, the actual time dependence of its *generalized* coordinates $\{q_i(t)\}$ minimize the action on the way from state 1 to state 2, that is the action path that the system choose will always be the minimal path, such that

$$S = \int_{t_1}^{t_2} \mathcal{L}(q(t), \dot{q}(t), t) dt, \quad q \equiv \{q_i\}$$

is minimum, hence must satisfy the Euler-Lagrange equation. One of such is the shortest path problem we have encountered in our example of the calculus of variation. Up to now, want can then ask about the reason why Lagrangian mechanics depends on the Hamiltonian principle (or why it is formulated as such). If we are to see the Lagrangian $\mathcal L$ as a somewhat energy functional of the system, then we can then interpret the integral $\mathcal S$ as the total effect of such energy function has on the given system, assuming that all information has been proxied by the energy functional of Lagrangian. Then, Hamiltonian's principle only states that the path that they take – or the real world takes, will be the one where the action is the least possible. This might not be clear for now, and surely it is for me, but perhaps it can be there to be dedicated in another post.

Some properties we can cite for the Lagrangian can be then conducted, which will be helpful in formalising the consequences of the Lagrangian formulation. First, the Lagrangian is independent of space and time. That is, the Lagrangian at this position, and at that position, as long as it is the same system, will not change. And secondly, it also does not depend on the direction of the system. This is all because we are indeed, still treating the Lagrangian in an inertial reference frame. Intrinsic of the Lagrangian, on the other hand, includes the property of a stationary point – subtle variations of the system won't change the Lagrangian by much of its least action; and secondly, it possesses the linearity property, that is, $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$, for all Lagrangians of interest. We will see how this is done in the latter sections.

2.3.3 Lagrangian of free mass (unconstrained motion)

Consider a particle moving unconstrained in three dimensions. They are not subjected to anything (short of a potential). Then, the Lagrangian \mathcal{L} can be said to only be determined on the kinetic energy T of the particle. That is, $\mathcal{L} = T$. So, how do we solve this particular problem?

We will begin this section with an alternative approach to forming the Lagrangian in this case. Hopefully, it still comes around to the above formation, just a bit not so out-of-context derivation as it is. Because the Lagrangian depends on the kinetic energy, apparently, it means it, *perhaps* depends on the velocity of the particle. But we remember that the Lagrangian is equivalent for all direction - which makes the velocity being independent of the Lagrangian. Except for the magnitude. We then can say that the Lagrangian depends on v^2 , of the squared magnitude of the velocity. That is, $\mathcal{L}(v^2)$. This dependency can then be expressed as

$$\mathcal{L}(v^2) = av^2$$

where a is an arbitrary constant. If we based off ourselves with the Galilee transformation, this choice also makes sense, because with this choice, the transformation of the Lagrangian from an

inertial frame to another inertial frame, it will stay the same or at least with very small deviation (I will write about this later, please).

For a, usually, we take it as m/2. It is also pretty evidential, somewhat, because we said that it only have kinetic energy. Then the Lagrangian is formulated by:

$$\mathcal{L} = T = \frac{1}{2}m\dot{\vec{r}}^2 = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$

for a 3-dimensional system in the Cartesian coordinates. If we only take the foremost expression, and apply it to the Euler-Lagrange equation, it gives

$$\frac{d}{dt}m\vec{v} = 0$$

which is indeed $m\vec{a}=0$. This fits the description of a free particle in an inertial frame. For spherical coordinate, you can express it as:

$$\mathcal{L} = \frac{m}{2}(\dot{r}^2 + r^2\dot{\varphi}^2 + \dot{z}^2)$$

And in the spherical coordinate:

$$\mathcal{L} = \frac{m}{2}(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin\theta^2\varphi^2)$$

If you get it a potential U(r), the Lagrangian will only change by (given the Cartesian coordinates):

$$\mathcal{L} = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + U(x, y, z)$$

In general, it holds for all generalized coordinates.

2.3.4 Multiple particles in actions

For an interacting system of multiple particles, we can then get the expression to be enumerated:

$$\mathcal{L} = \sum_{i=1}^{n} \frac{1}{2} m_i v_i^2 - U(x_1, y_1, z_1, \dots, x_n, y_n, z_n)$$
 (2.3)

As usual, the force on the two particles are $F_i = -\nabla_i U$. Newton's second law then can be applied to each particle and yields the equations of momentum and force using the Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial q_1} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q_1}, \quad \dots \quad , \frac{\partial \mathcal{L}}{\partial q_n} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial q_n}$$
 (2.4)

which is equivalent to, for each particle present in the system (we currently assume the Cartesian reference frame),

$$m_i \frac{d}{dt} \mathbf{v}_i = \frac{\partial U}{\partial x}, m_i \frac{d}{dt} \mathbf{v}_i = \frac{\partial U}{\partial y}, m_i \frac{d}{dt} \mathbf{v}_i = \frac{\partial U}{\partial z}$$
 (2.5)

which are just also variations of Newton's second law $F_i = m\ddot{x} = \dot{p}_i$. This then is repeated for all particles.

These equations then imply that the integral

$$S = \int_{t_1}^{t_2} \mathcal{L} \, dt \tag{2.6}$$

is stationary. Also notice that we have to get \vec{v} instead because the magnitude squared is cancelled out. It is also interestingly, the Lagrangian derivation form of the Newton's second law for multi-particle interactions of a system. If we do not wish to use Cartesian, then we can go for any generalized coordinate system, and the result will still hold, no matter the case for the generalized coordinates. Though often this is preferably not included as a proof, we would try to tackle on this for our own, most likely in the setting of multiple particles in free actions. Note that our formulation is conducted in the inertial reference frame.

For a generalized coordinate system, then, we can use a trick of which we express the generalized system into the Cartesian frame. That is, for particle a, then

$$x_a = f_a(q_1, q_2, \dots, q_S), \quad \dot{x}_a = \sum_k \frac{\partial f_a}{\partial q_k}$$
 (2.7)

where f_a is the respective transformation that gives the expression for x_a from the generalized coordinate. Do this for all the axis (x, y, z), for f_{ax} , f_{ay} , f_{az} . Recall the Lagrangian in Cartesian coordinate, then we have:

$$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{n} m_i (\dot{x_i}^2 + \dot{y_i}^2 + \dot{z_i}^2) - U(q_1, \dots, q_S)$$

$$= \frac{1}{2} \sum_{i=1}^{n} m_i \left[\left(\sum_k \frac{\partial f_{ix}}{\partial q_k} \dot{q}_k \right)^2 + \left(\sum_k \frac{\partial f_{iy}}{\partial q_k} \dot{q}_k \right)^2 + \left(\sum_k \frac{\partial f_{iz}}{\partial q_k} \dot{q}_k \right)^2 \right] - U(q_1, \dots, q_S)$$
(2.8)

Now, set each of the inner sum component as:

$$\frac{\partial f_{ix}}{\partial q_k} \dot{q}_k = a_{ik}, \quad \frac{\partial f_{iy}}{\partial q_k} \dot{q}_k = b_{ik}, \quad \frac{\partial f_{iz}}{\partial q_k} \dot{q}_k = c_{ik}$$

We reduce the sum to:

$$\mathcal{L} = \frac{1}{2} \sum_{i=1}^{n} m_{i} \left[\left(\sum_{k} a_{ik} \right)^{2} + \left(\sum_{k} b_{ik} \right)^{2} + \left(\sum_{k} c_{ik} \right)^{2} \right] - U(q_{1}, \dots, q_{S})$$

$$= \frac{1}{2} \sum_{i=1}^{n} m_{i} \left[\sum_{k} a_{ik}^{2} + \sum_{k} b_{ik}^{2} + \sum_{k} c_{ik}^{2} + 2 \sum_{k < j} a_{ik} a_{ij} + 2 \sum_{k < j} b_{ik} b_{ij} + 2 \sum_{k < j} c_{ik} c_{ij} \right]$$

$$- U(q_{1}, \dots, q_{S}) \tag{2.9}$$

Up to this point, you can then realize that we can substitute back the terms a_{ik} , b_{ik} , c_{ik} inside. Then, we have the following expansion:

$$\sum_{k} a_{ik}^2 = \sum_{k} \left(\frac{\partial f_{ix}}{\partial q_k} \right)^2 \dot{q}_k^2 \tag{2.10}$$

$$\sum_{k} b_{ik}^{2} = \sum_{k} \left(\frac{\partial f_{iy}}{\partial q_{k}} \right)^{2} \dot{q}_{k}^{2} \tag{2.11}$$

$$\sum_{k} c_{ik}^2 = \sum_{k} \left(\frac{\partial f_{iz}}{\partial q_k}\right)^2 \dot{q}_k^2 \tag{2.12}$$

$$\sum_{k < j} a_{ik} a_{ij} = \sum_{k < j} \left(\frac{\partial f_{ix}}{\partial q_k} \right) \left(\frac{\partial f_{ix}}{\partial q_j} \right) \dot{q}_k \dot{q}_j \tag{2.13}$$

$$\sum_{k < j} b_{ik} b_{ij} = \sum_{k < j} \left(\frac{\partial f_{iy}}{\partial q_k} \right) \left(\frac{\partial f_{iy}}{\partial q_j} \right) \dot{q}_k \dot{q}_j \tag{2.14}$$

$$\sum_{k < j} c_{ik} c_{ij} = \sum_{k < j} \left(\frac{\partial f_{iz}}{\partial q_k} \right) \left(\frac{\partial f_{iz}}{\partial q_j} \right) \dot{q}_k \dot{q}_j \tag{2.15}$$

(2.16)

Substitute all of this into the tray, well..., for the kinetic energy T of the Lagrangian, we have:

$$T = \frac{1}{2} \sum_{i=1}^{n} m_i \left(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2 \right)$$

$$= \frac{1}{2} \sum_{i=1}^{n} m_i \left[\sum_{k} \left(\left(\frac{\partial f_{ix}}{\partial q_k} \right)^2 + \left(\frac{\partial f_{iy}}{\partial q_k} \right)^2 + \left(\frac{\partial f_{iz}}{\partial q_k} \right)^2 \right) \dot{q}_k^2$$

$$+ 2 \sum_{k \le i} \left(\frac{\partial f_{ix}}{\partial q_k} \frac{\partial f_{ix}}{\partial q_j} + \frac{\partial f_{iy}}{\partial q_k} \frac{\partial f_{iy}}{\partial q_j} + \frac{\partial f_{iz}}{\partial q_k} \frac{\partial f_{iz}}{\partial q_j} \right) \dot{q}_k \dot{q}_j$$
(2.17)

Realize that you have two types of term, the diagonal terms where k=j (since it is a square, so two repeated terms), and the non-diagonal terms, we can then group them together into a sum, that is:

$$T = \frac{1}{2} \sum_{k=1}^{s} \sum_{i=1}^{s} \sum_{k=1}^{n} m_{i} \left(\frac{\partial f_{ix}}{\partial q_{k}} \frac{\partial f_{ix}}{\partial q_{j}} + \frac{\partial f_{iy}}{\partial q_{k}} \frac{\partial f_{iy}}{\partial q_{j}} + \frac{\partial f_{iz}}{\partial q_{k}} \frac{\partial f_{iz}}{\partial q_{j}} \right) \dot{q}_{k} \dot{q}_{j}$$
(2.18)

Now, we can simplify this form of the kinetic energy by considering a definite metric for the system. This is perhaps quite outlandish, suddenly, but simply speaking, now we are considering the metric space in which our particles, our system will operate. hence, consequentially, metric in this form will give us the relevant positional information, and the contributive mass of each particle subsequently. You can think about it as the contributing velocity, positional, and mass configuration of the system, in the generalized coordinate. You can reference this back to the original Cartesian/Descartes coordinate, though. Then, denote by $a_{ik}(q)$, we can set it as:

$$a_{jk}(q) = \sum_{i=1}^{n} m_i \left(\frac{\partial f_{ix}}{\partial q_k} \frac{\partial f_{ix}}{\partial q_j} + \frac{\partial f_{iy}}{\partial q_k} \frac{\partial f_{iy}}{\partial q_j} + \frac{\partial f_{iz}}{\partial q_k} \frac{\partial f_{iz}}{\partial q_j} \right)$$

and we call this the supposed Lagrangian metric for a multi-particle system. The system then is reduced to:

$$\mathcal{L} = \frac{1}{2} \sum_{k=1}^{s} \sum_{j=1}^{s} a_{kj}(q) \, \dot{q}_k \, \dot{q}_j - U(q_1, \dots, q_S) = \frac{1}{2} \sum_{k,j}^{s} a_{kj}(q) \, \dot{q}_k \, \dot{q}_j - U(q_1, \dots, q_S)$$

Which concludes our form of the Lagrangian. Under this form, however, also note that for a dynamical system of many particles, now U might, in circumstances, depends on time.

2.4 Lagrangian on constrained system

It is arguably then, one of the greatest strength of Lagrangian approach, is that it can handle systems that are constrained so that they cannot move arbitrarily in the space that they occupy.

This is most illustrated in the example of the *plane pendulum*, or the more difficult variation called the *double plane pendulum*. Working this out, it is perhaps then our interest to investigate those systems in earnest, to see the way or, *how long of an expression* can Newtonian formalism makes instead of Lagrangian.

2.4.1 An example

We then give the very, perhaps nominally famous example of the pendulum and double pendulum. The double pendulum consists of two masses m_1 and m_2 , connected by rigid weightless rods of length l_1 and l_2 , subject to gravity forces, and constrained by the hinges in the rods to move in a plane. We choose a coordinate system with the origin at the top suspension point, the x-axis as a horizontal axis in the plane of motion, and the y-axis pointing down (so that gravity forces have positive components). The single plane pendulum, a simpler case, has a single particle hanging from a rigid rod, hence the component m, l.

For the *constraints*, in the simple pendulum system, we have a single particle with position vector $\mathbf{r} = (x, y, z)$. There are two constraints present: oscillation in the (x, y)-plane, and it is always at a fixed distance from the suspension point. Mathematically,

$$z = 0, \quad |\mathbf{r}| = l \tag{2.19}$$

Usually, we would not consider the suspension point to be specified of coordinate. However, in certain setting like *plane pendulum with moving support* (or suspension), then it is then detrimental to at least specify the direction of free motion of the suspension part.

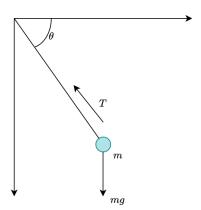


Figure 2.1: Diagram of a single pendulum with a single mass m and a rod of length ℓ connecting it.

The double pendulum, on the other hand, has two particles for N=2, with position vectors ${\bf r}_1, {\bf r}_2$ each with components (x_i,y_i,z_i) . There are four constraints, up from two: each particle moving in the (x,y)-plane, and each rod having constant lengths. These constraints can be expressed as:

$$z_1 = 0 (2.20)$$

$$z_2 = 0$$
 (2.21)

$$|\mathbf{r}_1| = l_1 \tag{2.22}$$

$$|\mathbf{r}_2 - \mathbf{r}_1| = l_2 \tag{2.23}$$

These constraints are *holonomic*, that is, constraints that are only algebraic relationships between the coordinates, and do not involve any "moving part" as derivative or inequalities. This is presented in the diagram of Figure 2.1.

holonomic

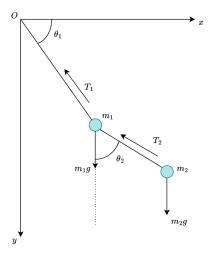


Figure 2.2: Diagram of a double pendulum with two masses: m_1 and m_2 , with their respective ℓ_1 connecting the origin to m_1 , and ℓ_2 connecting m_1 to m_2 .

In the single pendulum case, we only have *one particle*, hence N=1, hence three component coordinates of 3N=3. Since we now have two constraints, so m=2, we are left with n=3N-m=1, only one generalized coordinate. This is the angular position of the pendulum θ , which we then can write the position vector as

$$\mathbf{r} = l \cdot (\sin \theta, \cos \theta, 0) \tag{2.24}$$

To not be confused, here instead of writing the entire expression, each one for x,y,z, we denote the entire $(\sin\theta,\cos\theta,0)$ as a unit vector of such positional coordinate. Later on, kinematic and force analysis on the system of our plane pendulums can also remove 0, since it does not matter either way. Now, for the double pendulum again, we know that there should be only two generalized coordinates, sine there are 3N=6 coordinates. By the number of constraints being 4, so 3N-m=2 generalized coordinate. This is analogous to the two angular positions θ_1,θ_2 , which can express ${\bf r}_1,{\bf r}_2$ as

$$\mathbf{r}_1 = l_1(\sin \theta_1, \cos \theta_1, 0) \tag{2.25}$$

$$\mathbf{r}_2 = \mathbf{r}_1 + l_2(\sin\theta_2, \cos\theta_2, 0) \tag{2.26}$$

With this, we can analyse two components that specify the equation of motion later on - the *kinematic* and the *force* of the system.

Kinematic

For the singular pendulum, we can express velocity and acceleration vectors in terms of generalized coordinate as

$$\mathbf{r} = l(\sin \theta, \cos \theta, 0) \tag{2.27}$$

$$\dot{\mathbf{r}} = \mathbf{v} = l\dot{\theta}(\cos\theta, -\sin\theta) \tag{2.28}$$

$$\ddot{\mathbf{r}} = \mathbf{a} = l\ddot{\theta}(\cos\theta, -\sin\theta) - l\dot{\theta}^2(\sin\theta, \cos\theta) = l\ddot{\theta}\hat{\mathbf{v}} - l\dot{\theta}^2\hat{\mathbf{r}}$$
(2.29)

for the two unit vectors. The velocity vector \mathbf{v} is perpendicular to the position vector \mathbf{r} , which is the expression of the constraint $|\mathbf{r}| = l = \mathrm{const.}$ For the acceleration, there is the tangential and the centripetal acceleration terms, proportional to the velocity and to the inverted radial directions, respectively. For the double pendulum, we derive the same expressions for the first particle, albeit now it is a bit messier.

$$\mathbf{r}_1 = l_1(\sin \theta_1, \cos \theta_1) \tag{2.30}$$

$$\dot{\mathbf{r}}_1 = \mathbf{v}_1 = l_1 \dot{\theta}_1 (\cos \theta_1, -\sin \theta_1) \tag{2.31}$$

$$\ddot{\mathbf{r}}_1 = \mathbf{a}_1 = l_1 \ddot{\theta}_1 (\cos \theta_1, -\sin \theta_1) - l_1 \dot{\theta}_1^2 (\sin \theta_1, \cos \theta_1) \tag{2.32}$$

$$=l_1\ddot{\theta}_1\hat{\mathbf{v}}_1 - l_1\dot{\theta}_1^2\hat{\mathbf{r}}_1\tag{2.33}$$

and the second particle as:

$$\mathbf{r}_2 = \mathbf{r}_1 + l_2(\sin\theta_2, \cos\theta_2) \tag{2.34}$$

$$\dot{\mathbf{r}}_2 = \mathbf{v}_2 = \mathbf{v}_1 + l_2 \dot{\theta}_2 (\cos \theta_2, -\sin \theta_2) \tag{2.35}$$

$$\ddot{\mathbf{r}}_2 = \mathbf{a}_2 = \mathbf{a}_1 + l_2 \ddot{\theta}_2 (\cos \theta_2, -\sin \theta_2) - l_2 \dot{\theta}_2^2 (\sin \theta_2, \cos \theta_2)$$
 (2.36)

From here, we can already see the expression is very long. Combine them with forces, and we would have a lot of trouble managing all the terms - for the single simple problem.

Forces

In the single pendulum case, the forces on the particle are gravity and tension. Gravity is along the y-direction, or the direction of the gravitational acceleration g, and the tension is pointing towards the origin, along the direction of $-\mathbf{r}$:

$$\mathbf{F} = T \frac{-\mathbf{r}}{|\mathbf{r}|} + m\mathbf{g} = \frac{T}{l}\mathbf{r} + m\mathbf{g}$$
(2.37)

In the double pendulum, the forces on m_1 are the tension in the two rods, and gravity. The tension in the upper rod is along the direction $-\mathbf{r}_1$, the tension force on m_1 due to the lower rod is along the direction $\mathbf{r}_2 - \mathbf{r}_1$, so we can write the force \mathbf{F}_1 as

$$\mathbf{F}_{1} = T_{1} \frac{-\mathbf{r}_{1}}{|\mathbf{r}_{1}|} + T_{2} \frac{\mathbf{r}_{2} - \mathbf{r}_{1}}{|\mathbf{r}_{2} - \mathbf{r}_{1}|} + m_{1}\mathbf{g}$$

$$= \frac{T_{1}}{l_{1}} \mathbf{r}_{1} + \frac{T_{2}}{l_{2}} (\mathbf{r}_{2} - \mathbf{r}_{1}) + m_{1}\mathbf{g}$$

$$(2.38)$$

The forces on m_2 includes the tension in the lower rod and gravity, with the tension on m_2 being along the direction of $-(\mathbf{r}_2 - \mathbf{r}_1)$:

$$\mathbf{F} = T_2 \frac{-(\mathbf{r}_2 - \mathbf{r}_1)}{|\mathbf{r}_2 - \mathbf{r}_1|} + m_2 \mathbf{g} = \frac{T_2}{l_2} (\mathbf{r}_2 - \mathbf{r}_1) + m_2 \mathbf{g}$$
(2.39)

Newtonian analysis

In the single pendulum case, Newton's law is $\mathbf{F}=m\ddot{\mathbf{r}}$. Writing the two non-trivial components, we have:

$$m\ddot{\mathbf{r}} = F = -\frac{T}{l}\mathbf{r} + m\mathbf{g} \tag{2.40}$$

This is expanded to

$$ml\left(\ddot{\theta}(\cos\theta, -\sin\theta) - \dot{\theta}^2(\sin\theta, \cos\theta)\right) = -T(\sin\theta, \cos\theta) + mg(0, 1)$$
 (2.41)

We thus have two equations:

$$ml(\ddot{\theta}\cos\theta - \dot{\theta}^2\sin\theta) = -T\sin\theta$$
 (2.42)

$$-ml\left(\ddot{\theta}\sin\theta + \dot{\theta}^2\cos\theta\right) = -T\cos\theta + mg \tag{2.43}$$

Notice that although we only have one generalized coordinate θ , we have two equations. That is because the equation also have the magnitude of the tension as an unknown, so we have two equations for the two unknowns, θ and T. One particular observation can conclude that they are nonlinear, involving trigonometric functions, which is very, very hard to solve directly. We can, though, do this the easy way and use trigonometric identities. For example, multiplying Equation 2.42 by $\cos\theta$ and adding it with Equation 2.43 multiplied by $-\sin\theta$, we obtain a simpler equation for $\ddot{\theta}$. Using these identities, we can write the equation as:

$$l\ddot{\theta} - g\sin\theta \tag{2.44}$$

$$ml\dot{\theta}^2 = T \tag{2.45}$$

This cannot be solved analytically, though we can solve it numerically, or in small angle approximation, of which this particular differential equation would then again, be quite hard to reach with integration.

In the double pendulum case, we also proceed to do the same. However, by the time you increase the system dynamic up to two pendulums, the system gets insanely complex. Though the process is the same, we obtain the four equation of motions as:

$$l_1\ddot{\theta}_1 = (T_2/m_1)\sin(\theta_2 - \theta_1) - g\sin\theta_1$$
 (2.46)

$$l_1\dot{\theta}_1^2 = (T_1/m_1) - (T_2/m_1)\cos(\theta_2 - \theta_1) - g\cos\theta_1$$
(2.47)

$$l_2\ddot{\theta}_2 = -(T_1/m_1)\sin(\theta_2 - \theta_1) \tag{2.48}$$

$$l_2\dot{\theta}_2^2 = (T_2/m_2) + (T_2/m_1) - (T_1/m_1)\cos(\theta_2 - \theta_1)$$
(2.49)

Since there are no derivatives for T_1, T_2 , the best way to cast these equations for analytical or numerical solutions is to obtain two differential equations for θ_1, θ_2 without T_1, T_2 , and use their solution in expression for T_1, T_2 in terms of θ_1, θ_2 . From there, we obtain:

$$T_1 = -m_1 \frac{l_2 \ddot{\theta}_2}{\sin(\theta_2 - \theta_1)} \tag{2.50}$$

$$T_2 = m_1 \frac{l_1 \ddot{\theta}_1 + g \sin \theta_1}{\sin (\theta_2 - \theta_1)}$$
 (2.51)

We can now finally use these to obtain the form of our equations:

$$l_1 \dot{\theta}_1^2 = -\frac{l_2 \ddot{\theta}_2}{\sin(\theta_2 - \theta_1)} - \frac{l_1 \ddot{\theta}_1 + g \sin \theta_1}{\sin(\theta_2 - \theta_1)} \cos(\theta_2 - \theta_1) - g \cos \theta_1$$
 (2.52)

$$-l_1\dot{\theta}_1^2\sin(\theta_2 - \theta_1) = l_2\ddot{\theta}_2 + l_1\ddot{\theta}_1\cos(\theta_2 - \theta_1) + g\sin\theta_2 \tag{2.53}$$

It took a while for us to get to this point.

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Lagrangian analysis

Now, as we have been observing of the Newtonian analysis for both single pendulum and double pendulum, it is very long, complex and cumbersome, especially when it comes to counting forces and factors. Let's do it in the Lagrangian way.

In the **single pendulum** case, there is only one generalized coordinate, θ , so we want to write the Lagrangian in terms of θ , $\dot{\theta}$ and then derive the equation of motion as θ from the Lagrangian.

2.5 Generalized system in general

Consider now an arbitrary system of N particles, $\alpha = 1, ..., N$ with positions \mathbf{r}_{α} . We say that the parameters $q_1, ..., q_n$ are a set of **generalized coordinates** for the system if each position \mathbf{r}_{α} can be expressed as a function of $q_1, ..., q_n$, and possibly the time t, that is

$$\mathbf{r}_{\alpha} = \mathbf{r}_{\alpha}(q_1, \dots, q_n, t) \quad [\alpha = 1, \dots, N]$$
(2.54)

and conversely each q_i can be expressed in terms of the \mathbf{r}_{α} and possibly t,

$$q_i = q_i(\mathbf{r}_1, \dots, \mathbf{r}_N, t), \quad [i = 1, \dots, n]$$
(2.55)

Intuitively, this is pretty simple. In a constrained system, components is then related to each other such that their position is restricted by other generalize coordinate contributions. Conversely, the coordinate themselves can be specified, or expressed, in terms of calculating others coordinate of the system itself. An unconstrained system, will have its full coordinates (by the degree of freedom, which indicts restrictions on how many coordinates might ensue), and it will not be restricted by any means – hence effectively, all the generalized coordinate in such system is independent of each other,

$$q_i = q_i(0, 0, \dots, \mathbf{r}_i, \dots, 0, t)$$
 (2.56)

for example. Somehow, because of that, introducing degree of freedom early is somewhat unnecessary, because only now we would be using it. Nevertheless. In addition, we require that the number of the generalized coordinate n is the smallest number that allows the system to be parameterized this way. In our three-dimensional world, the number n of generalized coordinates for N particles is certainly no more than 3N, as established, though for constrained system the number would certainly be less. At this place, we would be required to brought up two notions about the constraints and their form. This will proceed as followed.

When the number of degree of freedom of an N-particle system in three dimensions is less than 3N, then we say it is *constrained*, or by kN for each dimension. If, furthermore, the number of degrees of freedom is equal to the number of generalized coordinates needed to describe the system's configuration, then is said to be **holonomic**. Holonomic systems are easier to treat than nonholonomic, and we would see why.

constrained system

Though, it is nice to also notice that what we have been doing comes down to the **positional features** in the more generalized coordinate system of the *reference frame* instead. Hence, we can say that, in a lot of cases, *nonholonomic systems* are inherently more complex because they have added, non-positional features strictly to the reference frame of the object in consideration. For example, to facilitate motions in three-dimension, one would simply need to get three coordinates, and hence they are also the degree of freedom, positionally. However, consider the makeshift name of the *degree of configuration*, then if the object is a ball, and we somehow add the requirement that their motions are dictated by rolling in 3D (not sure how that is, but you can imagine that as rolling a ball with variations of a hyperplane), then there exists another configuration called the *angular configuration* that indicate its orientation. Since the ball

is 'rolling' in three dimensions, then it needs three more generalized coordinates of the vertical and the two plane horizontal rotating orientation – in fact, these configurations are equal to the classification of symmetry group C_3 , hence brings the total of coordinate required to six. Evidently, this is a nonholonomic system for (x,y,z) specifying the level set z-hyperplane, and (ϕ_1,ϕ_2,ϕ_3) being orientation parameters.

Although nonholonomic systems certainly exist, they are more complicated to analyse than holonomic system. For any holonomic system with generalized coordinates q_1, \ldots, q_n and potential energy $U(q_1, \ldots, q_n, t)$, which may depend on t or not, the evolution in time is determined by the n Lagrange equations:

$$\frac{\partial \mathcal{L}}{\partial q_i} = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i}, \quad [i = 1, \dots, n]$$
(2.57)

where the Lagrangian $\mathcal L$ is defined as usual to be $\mathcal L=T-U.$

Chapter 3. Quantum mechanics

II. Research

A man who thinks all the time, has nothing except thoughts. If we want to do something, I would rather do it in practice $\frac{1}{2}$

Chapter 4. Quantum Well analysis - Expository

4.1 Note

This one is an expository research that I did in 2024 and 2025 for the topic of semiconducting theoretical analysis, typically of quantum well structure. Hence, you would be seeing a very specific type of quantum well that we have here.

4.2 What is quantum well?

All of the physics and devices in semiconductors, at most the basis of modern devices, are based on properties of direct gap semiconductors near the center of the Brillouin zone¹ being a Wigner-Seitz primitive cell in the reciprocal lattice²

Quantum wells are thin layered semiconductor structures in which we can observe and control many quantum mechanical effects. They derive most of their special properties from the quantum confinement of charge carriers (electrons and "holes") in thin layers (e.g 40 atomic layers thick) of one semiconductor "well" material sandwiched between other semiconductor "barrier" layers. They can be made to a high degree of precision by modern epitaxial crystal growth techniques. Many of the physical effects in quantum well structures can be seen at room temperature and can be exploited in real devices. From a scientific point of view, they are also an interesting "laboratory" in which we can explore various quantum mechanical effects, many of which cannot easily be investigated in the usual laboratory setting. For example, we can work with "excitons" as a close quantum mechanical analog for atoms, confining them in distances smaller than their natural size, and applying effectively gigantic electric fields to them, both classes of experiments that are difficult to perform on atoms themselves. We can also carefully tailor "coupled" quantum wells to show quantum mechanical beating phenomena that we can measure and control to a degree that is difficult with molecules.

A partial list of materials used for quantum well structures includes: III-V's - GaAs/GaAlAs on GaAs (Type I), GaSb/GaAlSb on GaSb (Type I), InGaAs/InAlAs on InP (Type I), InAs/GaSb (Type II), InGaAs/GaAs (Type I, strained); II-VI's - HgCdTe/CdTe, ZnSe/ZnMnSe (semi-magnetic), CdZnTe/ZnTe (Type 1, strained); IV-VI's - PbTe/PbSnTe; IV - Si/SiGe (strained)³.

¹The concept of a Brillouin zone was first developed by Léon Brillouin (1889-1969). Brillouin zones are polyhedra in reciprocal space in crystalline materials and are the geometrical equivalent of Wigner-Seitz cells in real space. Physically, Brillouin zone boundaries represent Bragg planes which reflect (diffract) waves having particular wave vectors so that they cause constructive interference.

²Every crystal structure has two lattices associated with it, the crystal lattice and the reciprocal lattice. A diffraction pattern of a crystal is the map of the reciprocal lattice of the crystal and a microscope structure is the map of the crystal structure. The meaning would be clarified later, as the footnote is too small

³Heterostructures for quantum well devices are constructed in three forms: the single-junction structures, often referred as simply heterostructures, the double - junction structures, mostly referred as quantum wells and - multijunction structures, called superlattices. Electron states in the structures are evaluated by assuming that the bulk band structures remain applicable for the constituents, even though the physical dimension in one or more directions may

For those materials there are indeed, requirement of determining the exact analytical results of any particular behaviour that one might want to predict, or to determine the distribution of specific structural landscape. However, such as rare by itself, and most of the time, we resort to numerical results by approximating the differential quantum equation. In a few different, well-constructed and well-designed structure however, such solution can be attained.

4.3 The dimensional Schrödinger equation

Given the wavefunction $|\psi(x)\rangle$, denoted more general as just $\psi(x)$ for time-independent case, we have the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \tag{4.1}$$

The Schrödinger equation then can be solved separably, as:

$$-\frac{h^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi, \quad \frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi \tag{4.2}$$

This is the case for consideration to time-independent equation, of the stationary state, as we have taken the canonical *separable solution*:

$$\Psi(x,t) = \psi(x)\varphi(t) \tag{4.3}$$

In case of non-specified V(x), we can only solve the differential equation which includes the time-dependent term:

$$\Psi(x,t) = \psi(x) \exp\left(-iE/\hbar\right) \tag{4.4}$$

As illustrated, we often have such assumption about the system that our solution are indeed *separable*, which allows us to separate all the dimensional terms, and time-dependent to be multiplicative under the quantum formalism. We would be coming back to this later, but for now, let's see how we can then solve some potential of multiple dimension using the above method.

4.4 The 3-dimensional case

Typically, the Schrödinger is stated in its one-dimensional form, concerning of only a single axis. This can be extended to the three-dimension space, with an added independent evolutionary variable t of time. We would then see how the Schrödinger equation can change the interpretation of **particle in a box** to higher dimensions. Because we are operating in higher dimensional space, we would use the Laplace operator $\nabla^2 \psi(\vec{r})$, for $\vec{r}=(x,y,z)$ instead, expressed by

$$\nabla^2 \psi(\vec{r}) = \left(\frac{\partial^2 \psi(\vec{r})}{\partial x} + \frac{\partial^2 \psi(\vec{r})}{\partial x} + \frac{\partial^2 \psi(\vec{r})}{\partial x}\right) \tag{4.5}$$

Hence, the Schrödinger equation turns into

$$-\frac{h^2}{2m} \left(\frac{\partial^2 \psi(\vec{r})}{\partial x} + \frac{\partial^2 \psi(\vec{r})}{\partial x} + \frac{\partial^2 \psi(\vec{r})}{\partial x} \right) + V\psi(\vec{r}) = E\psi(\vec{r})$$
 (4.6)

The easiest way to solve this, is having the wavefunction defined as the product of individual function for each independent variable (separable of variables technique). This is convenient,

be comparable to the lattice constant. Electron states in the structures are obtained by solving the wave equation for the potential distributions in the structure by using the bulk physical constants and by applying the so-called effective mass approximation and suitable boundary conditions

although there might be cases where this is not possible. Then, the wavefunction can be separated to:

$$\psi(x, y, z) = X(x)Y(y)Z(z) \tag{4.7}$$

This is applicable, for example, between the equation of state for such case in which low-dimensional system is considered, for example, 1-dimensional restriction only, then we can effectively want to have the wavefunction in the form

$$\psi(x, y, z) = \psi_{\perp}(x, y)R(z)$$

with restriction in the z axis. We would first try to find the solution of equation 7. We have:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{X} \frac{\partial^2 X}{\partial x^2} \quad \frac{\partial^2 \psi}{\partial y^2} = \frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} \quad \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{Z} \frac{\partial^2 Z}{\partial z^2}$$
(4.8)

plugging this into (6), we gain:

$$\left(-\frac{\hbar}{2mX}\frac{\partial^2 X}{\partial x^2}\right) + \left(-\frac{\hbar}{2mX}\frac{\partial^2 X}{\partial x^2}\right) + \left(-\frac{\hbar}{2mX}\frac{\partial^2 X}{\partial x^2}\right) = E - V(r)$$

For V(r) = 0, i.e. the free particle, this turns into only

$$\left(-\frac{\hbar}{2mX}\frac{\partial^2 X}{\partial x^2}\right) + \left(-\frac{\hbar}{2mX}\frac{\partial^2 X}{\partial x^2}\right) + \left(-\frac{\hbar}{2mX}\frac{\partial^2 X}{\partial x^2}\right) = E$$
(4.9)

Another way to obtain this relative result and make use of it for the next up potential well, is as the following. We regard the two-dimensional problem, that is, the potential lies only on one singular axis, and others are free, of which then for the three-dimensional case is:

$$-\frac{\hbar}{2m}\left(\frac{\partial^2 \psi(x,y,z)}{\partial x^2} + \frac{\partial^2 \psi(x,y,z)}{\partial y^2} + \frac{\partial^2 \psi(x,y,z)}{\partial z^2}\right) + U(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

For two-dimensional, z-constrained wave function system, we have the following separable exposition:

$$\psi(x, y, z) = \psi_{\perp}(\vec{r}_{\perp})\psi_n(\vec{r})\varphi(t)$$

Where $\psi_{\perp}(\vec{r}_{\perp})$ is the wavefunction of the waveform along the non-restricted, free space of the Oxy plane, while $\psi_n(\vec{r})$ is the restricted waveform along the z axis. Hence, we have:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi(x, y, z)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z)}{\partial y^2} \right) + U(x, y)\psi(x, y) = E\psi(x, y) \quad (1)$$

and

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi(x, y, z)}{\partial z^2} \right) + U(z)\psi(z) = E\psi(z) \quad (2)$$

Here, we substitute U(z), and first received the equation for certain form of

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi(x, y, z)}{\partial z^2} \right) + \left(\frac{1}{2} m_e \omega_z^2 x^2 \right) \psi(z) = E \psi(z)$$

Which brings us to the formulation of our well of interest.

4.4.1 The infinite square cube

The most simple case of quantum physics, when extended to 3D, would be the elementary space of an **infinite square well**. Indeed the following potential configuration:

$$V(\vec{r}) = \begin{cases} 0 & 0 \le x, y, z \le L_x, L_y, L_z \\ \infty & \text{otherwise} \end{cases}$$
 (4.10)

which would seems like to be the case, is indeed, called an *infinite square cube* that restricts a space by a three-dimensional region cut.

Since energy is constant, we need a working constant to then figure out the solution of the system. That means that each dimension need to have a working constant on its own. for example,

$$-\frac{\hbar^2}{2mX}\frac{d^2X}{dx^2} = \epsilon_x$$

$$\Leftrightarrow \frac{d^2X}{dx^2} = -\frac{2m}{\hbar^2}\epsilon_x$$

$$0 = \frac{d^2X}{dx^2} + \frac{2m}{\hbar^2}\epsilon_x$$

Applying this for all term, we have:

$$\partial \vec{E} = \begin{bmatrix} \frac{\partial^2(X)}{\partial x^2} + \frac{2m}{\hbar^2} \epsilon_x = 0\\ \frac{\partial^2(Y)}{\partial y^2} + \frac{2m}{\hbar^2} \epsilon_y = 0\\ \frac{\partial^2(Z)}{\partial z^2} + \frac{2m}{\hbar^2} \epsilon_z = 0 \end{bmatrix}$$
(4.11)

Where the term $\epsilon_{x,y,z}$ is as:

$$\vec{E} = \begin{bmatrix} \epsilon_x \\ \epsilon_y \\ \epsilon_z \end{bmatrix} \longrightarrow \langle \vec{v}, \vec{1} \rangle = \epsilon_x + \epsilon_y + \epsilon_z = E \tag{4.12}$$

This reduce everything into one variable, single dimension result:

$$\frac{\partial^2 X}{\partial x^2} = \frac{2m}{\hbar^2} E_x X = 0 \approx \frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\hbar^2} \psi$$

of which λ is the De Broglie wavelength.

The boundary condition now is easy to solve, and thus we have the ladder of changing linear combination, $n=1,\ldots,\infty$.

Using normalization constant

$$A_{x,y,z} = \sqrt{\frac{2}{L_{x,y,z}}} (4.13)$$

we gain the form of the x-directive:

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{L_x}} \sin \frac{n\pi x}{L_x} & \text{if } 0 \le x \le L\\ 0 & \text{if } L < x < 0 \end{cases}$$

and apply this to all other axis,

$$X(x) = \sqrt{\frac{2}{L_x}} \sin \frac{n\pi x}{L_x} \tag{4.14}$$

$$Y(y) = \sqrt{\frac{2}{L_y}} \sin \frac{n\pi y}{L_y} \tag{4.15}$$

$$Z(z) = \sqrt{\frac{2}{L_z}} \sin \frac{n\pi z}{L_z} \tag{4.16}$$

For each constant, we derive from the De Broglie's constant:

$$\epsilon_{x} = \frac{n_{x}^{2}h^{2}}{8mL_{x}^{2}}, \ \epsilon_{y} = \frac{n_{y}^{2}h^{2}}{8mL_{y}^{2}}, \ \epsilon_{z} = \frac{n_{z}^{2}h^{2}}{8mL_{z}^{2}}$$

which gives us the accurate representation, if possible, for those vaue inside the wavefunction form. Plugging everything (almost) into (7), we gain:

$$\psi(r) = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right)$$

$$= \sqrt{\frac{8}{V}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right)$$
(4.17)

with total energy

$$E_{n_x,n_y,n_z} = \frac{h^2}{8m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$
 (4.18)

4.5 The quantum well

We are taking on researches of solving the fundamental case of a low-dimensional semiconductor. By this, we mean that at the microscopic scale, we restrict its movement to be free only in sub-dimensions, less than 3. For example, our task on the half-parabolic, non-additive, antisymmetric quantum well which serves to facilitate this kind of restriction is:

$$U(z) = \begin{cases} S_0 & z < a \\ \frac{1}{2} m_e \omega_z^2 z^2 & a \le z \le b \\ S_0 & z > b \end{cases}$$
 (4.19)

Where m_e is the mass of electron, ω_z is the angular momentum at z, for z changing in [a, b]. A reduced form of this potential well is to treat its boundary as *infinite bound*, that is, we can rewrite the thing as

$$U(z) = \begin{cases} +\infty & z < a \\ \frac{1}{2} m_e \omega_z^2 z^2 & a \le z \le b \\ +\infty & z > b \end{cases}$$
 (4.20)

which effectively makes the wavefunction to be restricted to only the portion of space [a,b]. This quantum well is often called the asymmetric, half-parabolic but *non-additive* quantum well. The reason for the term non-additive is because of the complement term that would be later addressed

For wavefunction in quantum mechanics, its evolution in time, or the dynamic, is governed by the Schrödinger equation. This equation links the Hamiltonian operator to the energy operator together. For now, the **Hamiltonian** is the operator that describes the energy of particles, for it is the sum of kinetic and potential energy operators, $H=-E_k+V(x)$. By letting both the Hamiltonian and the energy operator act on the wave function, we define the behaviour of the particle as $H\Psi(x,t)=E\Psi(x,t)$ In such, we gain the following expanded form of the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x,t) + V(x)\Psi(x,t) = i\hbar\frac{d}{dt}\Psi(x,t)$$

Which is now the *time-dependent Schrödinger wave equation*. To solve this quantum well, first reciting the Schrödinger equation with Laplacian operator:

$$-\frac{\hbar}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + U(x, y, z) \psi(x, y, z) = E\psi(x, y, z) \tag{4.21}$$

we can separate the wavefunction as:

$$\Psi(Oxyz,t) = \psi_{\perp}(\vec{r}_{\perp})\psi_n(\vec{r})\varphi(t) \tag{4.22}$$

Where $\psi_{\perp}(\vec{r}_{\perp})$ is the wavefunction of the waveform along the non-restricted, free space of the Oxy plane, while $\psi_n(\vec{r})$ is the restricted waveform along the z axis. The result along the free space is easier, since it is just the free particle quantum system, which has elementary results. The z axis though, is a problem, since its bound is pretty complex on the side of asymmetry.

The inner well can then be specified along the z axis as.

$$\mathcal{O}\left(S_0, \frac{1}{2}m_e\omega_z^2 z^2\right) \tag{4.23}$$

It is realized from the fact that The well depends on the conductor band interface difference between the two, hence it must start somewhere from the boundary itself. The various forms can be

$$S_0 \pm \frac{1}{2} m_e \omega_z^2 z^2 {(4.24)}$$

or

$$S_0 \cdot \left[\frac{1}{2} m_e \omega_z^2 z^2 \right], \quad n \in \{-1, 1\}$$
 (4.25)

For formality and causality, the second case is more likely to be the form inside the well structure of two conducting bands, hence we will go with the multiplicative case.

4.5.1 Related formulation

When dealing with quantum well or other structures in quantum mechanics, typically specified by their potential, it is of best interest that we familiarize ourselves with the reduced, simple form of some of the potential often met. This includes in the following list of:

- 1. Symmetric potential.
- 2. Asymmetric potential.
- 3. Parabolic potential.
- 4. Free parabolic/symmetric potential.
- 5. (In)finite square well.
- 6. (In)finite parabolic well.
- 7. Semi-parabolic well.
- 8. Semi-parabolic asymmetric well (A composition between parabolic and asymmetric)

Note that this includes both the *finite potential well* and the infinite one. Usually, infinite is often endowed upon the problem setting, especially if the formulation and scenario permits such. This is because if it is "borderline" infinite, or just infinite in general, then the wavefunction of the particle of interest will lie entirely in the potential region, with almost (not impossible) a hundred percent accuracy of inclusion. This is why, if able, we would generally consider the boundary to be infinite or acting as one.

4.5.2 Symmetric infinite square potential

Of the first feature, of symmetric potential well, it is a box of length L with its left-hand edge placed at x-coordinate – L/2. The wave function is set to 0 outside the box.

For a particle in an infinite spare well of length L centred at the origin, demonstrated above, the potential V(x) is given by

$$V(x) = \begin{cases} 0 & -\frac{L}{2} \le x \le \frac{L}{2} \\ \infty & \text{otherwise} \end{cases}$$
 (4.26)

Since the particle cannot be found outside the well, the wave function $\Psi(x)$ outside the well is set to zero with

$$\Psi(x) = 0$$
 when $x < -\frac{L}{2}$ or $x > \frac{L}{2}$

In order to have $\Psi(x)$ remain continuous, the Dirichlet boundary conditions are set as

$$\Psi\left(-\frac{L}{2}\right) = \Psi\left(\frac{L}{2}\right) = 0$$

After this, we can solve the potential by equation (1) as:

$$\Psi(x) = A\cos kx + B\sin kx \qquad A, B \in R \tag{4.27}$$

with

$$k = \sqrt{\frac{2mE}{\hbar}}$$

Applying the boundary conditions from Eq (2) to Eq (3), we can have

$$A\cos k\left(\frac{L}{2}\right) + B\sin k\left(\frac{L}{2}\right) = 0$$

with

$$k_n = \frac{n\pi}{L}$$

from Eq (4) and Eq (6), the energy E is quantized as

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$
 $n = 1, 2, 3, \dots$

Normalizing this wavefunction is defined by using the boundary condition:

$$\int_{-L/2}^{L/2} |\psi_n(z)|^2 dz = 1 \tag{4.28}$$

For n even, the cosine term takes in place, while for the odd case, the sine term takes place. Hence,

$$A^{2} \int_{-L/2}^{L/2} \sin^{2}\left(\frac{n\pi}{L}z\right) dz = 1, \quad n \text{ is even}$$
 (4.29)

$$B^2 \int_{-L/2}^{L/2} \cos^2\left(\frac{n\pi}{L}z\right) dz = 1, \quad n \text{ is odd}$$
 (4.30)

The normalization results in

$$\Psi_{n_o}(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \cos\left(\frac{n\pi}{L}x\right) \qquad n = 1, 3, 5 \dots$$

and

$$\Psi_{n_e}(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi}{L}x\right) \qquad n = 2, 4, 6...$$

Handling this in the case of 3-dimensional potential, restricted of the z axis, and the form

$$\Psi(\vec{r}) = \varphi(t)e^{ik_{\perp}r_{\perp}}\psi_n(z) \tag{4.31}$$

thereby turns into

$$\Psi(\vec{r},t) = \underbrace{e^{-iEt/\hbar}}_{\text{time}} \times \underbrace{\sqrt{\frac{2}{L}} \left[\sin\left(\frac{n\pi}{L}z\right) + \cos\left(\frac{n\pi}{L}z\right) \right]}_{\text{Restricted axis}} \times \underbrace{Ae^{ik_{\perp}x_{\perp}}}_{\text{Free plane}}$$
(4.32)

The two normalization term A and $\sqrt{2/L}$ can be realized by superposing them, but for the free particle, it is troublesome since we need to solve the equation

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \vartheta(k)e^{ikx} dk$$
 (4.33)

such that the normalization condition $I(\psi_{\perp}(x))_{\mathbb{R}}=1$ as always.

4.5.3 Asymmetric Potential

To continue after covering up the symmetric potential well, here will be the figure that demonstrates the asymmetric potential well, which is a box length L with its left-hand edge placed at the origin. The wave function is set to zero outside the infinite boundaries

For a particle in an infinite square well with its left-hand edge at the origin, as seen from the figure above, the potential V(x) is defined as

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le L \\ \infty, & \text{otherwise} \end{cases}$$
 (4.34)

Once again, the wave function $\Psi(x)$ outside the well is set to zero with

$$\Psi(x) = 0$$
 when $x < 0$ or $x > L$

In order to have $\Psi(x)$ remain continuous, the Dirichlet boundary conditions are set as

$$\Psi(0) = \Psi(L) = 0$$

No restriction for continuity is made on $\frac{d\Psi(x)}{dx}$ at the boundary.

Using the same method to solve the case of time-independent Schrödinger equation for the potential on the symmetrical potential well, we have the result as

$$\Psi(x) = A\cos kx + B\sin kx \quad A, B \in \mathbb{R}$$
 (4.35)

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Applying the boundary condition $\Psi(0) = 0$ eliminates the constant A which leaves

$$\Psi(x) = B\sin kx$$

In order for $\Psi(L) = 0$, then $kL = n\pi$ thereby giving

$$k_n = \frac{n\pi}{L}$$
, with $n = 1, 2, 3, \dots$ (4.36)

From the energy E is quantized as

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

The constant B is found by normalizing $\Psi(x)$ as

$$\int_0^L |\Psi(x)|^2 dx = 1$$

which gives

$$B = \sqrt{\frac{2}{L}}$$

Finally, the wave solution for the particle in the infinite square well is given by

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$
 $n = \pm 1, \pm 2, \pm 3, \dots$

4.5.4 Semi-parabolic potential, I

In literature, we have the functional form of a semi-parabolic confining potential V(z), due to the difference of conduction band edge (as for quantum well which is usually created in an electrical structure of such – molecular-beam-epitaxy and related deposition):

$$V(z) = \begin{cases} V_S \left(\frac{z}{d}\right)^2 & 0 < z \le d \\ \infty & z \le 0 \end{cases}$$
 (4.37)

Per description as above cases, we can also partially state it as **asymmetric** of the central axis as well. Here, d is the quantum well width, V_S is the conduction band offset at interface.

The motion of an electron in the xy-plane is described in the weak-coupling approximation the coupling here likely refers to the **coupling constant**, the number that determines the strength of the force exerted in an interaction between static bodies to the charges of the bodies. In QFT, with a coupling g, if g is much less than 1, the theory uis said to be **weakly coupled**, the reverse is then **strongly coupled**; whereas the motion of the electron along the z-axis is governed by the potential V(z), therewithal the wavefunction and energy spectrum are determined from a solution of the Schrödinger equation:

$$\frac{\mathrm{d}^2 \varphi(z)}{\mathrm{d}z^2} + \frac{2m}{\hbar^2} \left(\bar{\epsilon} - \frac{1}{2} m \omega_s^2 z^2 \right) \varphi(z) = 0 \tag{4.38}$$

where

$$\omega_s = \frac{1}{d} \sqrt{\frac{2V_S}{m}} \tag{4.39}$$

is the frequency of the semi-parabolic potential in the quantum well, $\bar{\epsilon} = \epsilon - \epsilon \perp$.

Under the effective mass approximation and the envelope wavefunction approach, the eigenfunctions and eigenenergies (defined with the true sub-band energies and wavefunctions) are the solution of the Schrödinger equation.

From the boundary conditions for the wavefunction, such that

$$\varphi(z) = \begin{cases} 0 & z = 0 \\ 0 & z = d \end{cases} \tag{4.40}$$

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such that the wavefunction vanishes after reaching the boundary. We obtains the condition from such, that

$$\frac{d}{2\hbar}\sqrt{2mV_S} \gg 1\tag{4.41}$$

under which the solution of the Schrödinger equation for a semi-parabolic quantum well, infinite on the left and finite on the right, is given as:

$$\epsilon = \hbar\omega_s \left(2n + \frac{3}{2}\right), \quad \varphi_n(z) = A_n \exp\left(-\frac{\beta z^2}{2}\right) I_{2n+1} \left(\beta z + 1\right)$$
(4.42)

and the form of the wavefunction is as such:

$$\varphi_n(z) = A_n \exp\left(-\frac{\beta z^2}{2}\right) H_{2n+1}[(\beta z + 1)] \tag{4.43}$$

where

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \tag{4.44}$$

and $H_{2n+1}[(\beta z+1)]$ is the Hermite polynomial, and n is the quantum number. The explicit derivation needs to be taken into account, though we would not be concerned of such until further date (or at least in another exposition).

4.6 Solution draft

Now, after some investigations of related well, we note the following of interest:

1. The Schrödinger equation can be written as the *homogeneous*, *second order differential equation* in the case of mono-axis *z*:

$$-\frac{\hbar}{2m}\psi''(z) + Q(z)\psi(z) = 0$$
 (4.45)

Here, the differential equation is figured as *variable*, since the second factor Q(z) corresponds to the variable potential well inside the region [a, b]. In this case,

$$Q(z) = \frac{1}{2} m_e \omega_z^2 z^2 (4.46)$$

which closely resemble the harmonic quantum oscillator.

2. We remember the general form solution of the total solution to Schrödinger's equation is:

$$\Psi(z,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$
(4.47)

now, for when t = 0, we gain the initial condition of the wavefunction:

$$\Psi(z,0) = \sum_{n=1}^{\infty} c_n \psi_n(z)$$
(4.48)

3. The form of the potential well is somewhat difficult. We notice that it is asymmetric, the question is, how that asymmetry would be. The most basic structure available to this, then must be the curvature of which one side is at the section where Q'(z) = 0, i.e. the top maxima point of the potential curve.

4. To solve this complex situation, we might want to find the solution to the one-dimensional, non-boundary applicable potential. This case would have the symmetric parabolic potential. We then restrict on one side, the side of which means that we set up the system $[a,\infty)$. Similarly, we do it for $(\infty,b]$. Then we might come about to find out the solution to the general potential well interpretation.

This will be the partial guidance to solving the problem. Because we are recording the partial progress made, there will be a few attempts in obtaining such solution, as draft of getting closer to the answer. But first, thinking about it, it is the time to investigate its closer analogue, of the harmonic quantum oscillator.

4.7 The quantum harmonic oscillator

Oscillations are found in nature, in such things as electromagnetic waves, vibrating molecules and your bell, the flow of water, and the gentle back-and-forth sway of a tree branch. Previously, we deal with oscillation in a macroscopic way, such as spring and simple plane pendulum. Reusing such notion to microscopic scale, is a problem entirely different.

4.7.1 Classical harmonic oscillator

A simple harmonic oscillator is a particle or system that undergoes harmonic motion about an equilibrium position, such as an object with mass vibrating on a spring. Because quantum well exists within the restriction of a single dimensional figure, we would be considering the single-dimension variant only.

Suppose a mass moves back-and-forth along the x-dimension about the equilibrium position, x=0. In classical physics, the particle moves in response to a linear string $F_x=-kx$, where x is the displacement of the particle from its equilibrium position. The motion takes place between two turning points, $x\pm A$, where A denotes the amplitude of the motion. The position of the object varies periodically in time with angular frequency $\omega=\sqrt{k/m}$, which depends on the mass m of the oscillator and on the constant force k of the force, and be written

$$x(t) = A\cos(\omega t + \phi) \tag{4.49}$$

The total energy of an oscillator is the sum of its kinetic energy $K = mu^2/2$ and the elastic potential energy of the force $U(x) = kx^2/2$, which is

$$E = \frac{1}{2}mu^2 + \frac{1}{2}kx^2 \tag{4.50}$$

At the turning points $x=\pm A$, the speed of the oscillator is zero, therefore, at these point, the energy of the oscillation is solely in the form of its potential energy $E=kA^2/2$. Physically, it means that a classical oscillator can never be found beyond its turning points, and its energy depends only on how far the turning points are from its equilibrium position. The energy of a classical oscillator changes in a continuous way. The lowest energy that a classical oscillator may have is zero, which corresponds to a situation where an object is at rest at its equilibrium position. The zero-energy state of a classical oscillator simply means no oscillations and no motion at all (a classical particle sitting at the bottom of the potential well). When an object oscillates, no matter how big or small its energy may be, it spends the longest time near the turning points, because this is where it slows down and reverses its direction of motion. Therefore, the probability of finding a classical oscillator between the turning points is highest near the turning points and lowest at the equilibrium position.

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4.8 Solution

4.8.1 Attempt 1

The form of the inner well potential:

$$\frac{S_0}{2}m_e\omega_z^2 z^2 \tag{4.51}$$

contains the variations ω_z , which is the potential inner frequency, formulated as

$$\omega_z = \frac{1}{L} \sqrt{\frac{2S_0}{m_e}} \tag{4.52}$$

The inner Schrödinger equation becomes

$$-\frac{h^2}{2m_e}\frac{d^2\psi(z)}{dz^2} + \left(\frac{S_0}{2}m_e\omega_z^2 z^2\right)\psi = E\psi$$
 (4.53)

This can be simplified to

$$\frac{d^2\psi}{dz^2} = \frac{2m_e}{\hbar} \left(\frac{S_0 m_e \omega_z^2}{2} z^2 - E \right) \psi \tag{4.54}$$

that is

$$\frac{d^2\psi}{dz^2} = \left[\frac{S_0}{\hbar} (m_e \omega_z z)^2 - \frac{2Em_e}{\hbar}\right] \psi \tag{4.55}$$

Set $\mathcal{E}=(2Em_e)/\hbar$ and $\mathcal{Q}=(S_0m_e^2\omega_z^2)/\hbar$, we retract it to

$$\frac{d^2\psi}{dz^2} = \left[Qz^2 - \mathcal{E}\right]\psi\tag{4.56}$$

We note that by asymptotic analysis,

$$\lim_{z \to \pm \infty} (Qz^2 - \mathcal{E}) \approx Qz^2 \tag{4.57}$$

Hence

$$\lim_{z \to \pm \infty} \frac{d^2 \psi}{dz^2} \approx Q z^2 \psi \tag{4.58}$$

We can try then

$$\psi(z) = \psi_0 \exp{(\alpha z^2)/2}, \quad \alpha \equiv \sqrt{\frac{\hbar}{m\omega}}$$
 (4.59)

which leads to

$$\frac{d\psi}{dz} = \alpha z \psi \tag{4.60}$$

and

$$\frac{d^2\psi}{dz^2} = (\alpha + \alpha^2 z^2)\psi \approx \alpha^2 z^2 \psi \tag{4.61}$$

in the same limit. Compare this to the limit, we then have

$$\alpha^2 z^2 \psi = Q z^2 \psi \tag{4.62}$$

4.8.2 Attempt 2

Given that the potential depends only on z:

$$\left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2}\right) = 0, \quad \Rightarrow \quad V(x,y) = 0 \Rightarrow \Psi(x,y,z) = \psi(z)$$

Using the method of separation of variables, we arrive at the one-dimensional Schrödinger equation along the *z*-direction:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V(z)\right]\Psi(z)=E\Psi(z)$$

Where $\Psi(z)$ is the wavefunction and E is the corresponding energy in the z-direction. Case 0 < z < L

The equation becomes:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \frac{1}{2} m_e \omega_z^2 z^2 \right] \Psi(z) = E \Psi(z)$$

This is the equation of a one-dimensional harmonic oscillator.

Non-dimensionalization of the Equation

Multiply both sides of the equation by $\frac{2}{\hbar\omega_z}$:

$$\left[\frac{-\hbar}{m_e\omega_z}\frac{d^2}{dz^2} + \frac{m_e\omega_zz^2}{\hbar}\right]\Psi(z) = \frac{2E}{\hbar\omega_z}\Psi(z)$$

Let:

$$\alpha_z = \sqrt{\frac{\hbar}{m_e \omega_z}}, \quad \delta = \frac{z}{\alpha_z}$$

Then the equation becomes:

$$\left[-\frac{d^2}{d\delta^2} + \delta^2 \right] \Psi(\delta) = \frac{2E}{\hbar \omega_z} \Psi(\delta)$$

$$\Rightarrow \Psi''(\delta) + \left(\frac{2E}{\hbar\omega_z} - \delta^2\right)\Psi(\delta) = 0$$

Assume a solution of the form:

$$\Psi(\delta) \sim u(\delta)e^{-\frac{\delta^2}{2}}$$

Then:

$$\left[u''(\delta) - 2\delta u'(\delta) + \left(\frac{2E}{\hbar\omega_z} - 1\right)u(\delta)\right]e^{-\frac{\delta^2}{2}} = 0$$

(This can be simplified into the Hermite differential equation depending on the analysis.)

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This is the equation of the harmonic oscillator, and the solutions are Hermite polynomials multiplied by a Gaussian, with discrete energy levels:

$$E_n = \hbar\omega_z \left(n + \frac{1}{2} \right)$$

By normalizing and transforming the equation into the one-dimensional harmonic oscillator form, we determine the discrete energy spectrum and the asymptotic wavefunction shape in the parabolic region 0 < z < L.

Analysis Using Hermite Polynomials

Continuing from:

$$u''(\delta) - 2\delta u'(\delta) + \left(\delta^2 - 1 + \frac{2E}{\hbar\omega_z}\right)u(\delta) = 0$$

Simplifying:

$$u''(\delta) - 2\delta u'(\delta) + u(\delta) \left[\frac{2E}{\hbar \omega_z} - 1 \right] = 0$$

Let:

$$\lambda = \frac{2E}{\hbar\omega_z} - 1$$

Then the equation becomes:

$$u''(\delta) - 2\delta u'(\delta) + \lambda u(\delta) = 0$$

This is the Hermite differential equation with condition $\lambda = 2N$.

Therefore:

$$u(\delta) = H_N(\delta)$$

And:

$$\Psi(\delta) \sim u(\delta)e^{-\delta^2/2} = H_N(\delta)e^{-\delta^2/2}$$

Thus:

$$\Psi(\delta) = Ae^{-\delta^2/2}H_N(\delta)$$

With:

$$\delta = \frac{z}{\alpha_z}, \quad \alpha_z = \sqrt{\frac{\hbar}{m_e \omega_z}}$$

The wavefunction in terms of z is:

$$\Psi(z) = A \exp\left(-\frac{z^2}{2\alpha_z^2}\right) H_N\left(\frac{z}{\alpha_z}\right)$$

Boundary Condition at z=0

At z=0:

$$\Psi(0) = AH_N(0)$$

Depending on the boundary condition (e.g., infinite potential wall or symmetry/asymmetry), we choose appropriate N values (even or odd).

Since $H_N(0) = 0$ when N is odd, we have:

Even solutions (N = 0, 2, ...): discarded Odd solutions (N = 1, 3, ...): accepted

Wavefunction Normalization

Normalization condition:

$$\int_0^L |\Psi(z)|^2 dz = 1$$

Substitute the wavefunction:

$$\int_0^L A_N^2 \exp\left(-\frac{z^2}{\alpha_z^2}\right) H_{N+1}^2 \left(\frac{z}{\alpha_z}\right) dz = 1$$

Case N=0

$$A_0^2 \int_0^L \exp\left(-\frac{z^2}{\alpha_z^2}\right) dz = 1$$

Therefore:

$$A_0 = \left[-2e^{-\frac{L^2}{\alpha_z^2}} \cdot L + \alpha_z \sqrt{\pi} \operatorname{Erf}\left(\frac{L}{\alpha_z}\right) \right]^{-\frac{1}{2}}$$

 $\mathsf{Case}\ N=1$

$$A_1^2 \int_0^L \exp\left(-\frac{z^2}{\alpha_z^2}\right) H_3^2\left(\frac{z}{\alpha_z}\right) dz = 1$$

Result:

$$A_1^2 = \left\lceil \frac{16e^{-\frac{L^2}{\alpha_z^2}} \cdot L \cdot \left(-3\alpha_z^4 + \alpha_z^2 L^2 - 2L^4\right)}{\alpha_z^4} + 24\alpha_z\sqrt{\pi}\operatorname{Erf}\left(\frac{L}{\alpha_z}\right) \right\rceil^{-1}$$

Therefore:

$$A_1 = \left\lceil \frac{16e^{-\frac{L^2}{\alpha_z^2}} \cdot L \cdot \left(-3\alpha_z^4 + \alpha_z^2 L^2 - 2L^4\right)}{\alpha_z^4} + 24\alpha_z \sqrt{\pi} \operatorname{Erf}\left(\frac{L}{\alpha_z}\right) \right\rceil^{-\frac{1}{2}}$$

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Thus:

$$\psi_0(z) = \left[-2e^{-\frac{z^2}{\alpha_z^2}} \cdot L + \alpha_z \sqrt{\pi} \operatorname{Erf}\left(\frac{L}{\alpha_z}\right) \right]^{-\frac{1}{2}} \cdot e^{-\frac{z^2}{2\alpha_z^2}} \cdot H_1\left(\frac{z}{\alpha_z}\right)$$

This is the wavefunction for the case when the initial quantum number considered is N=0.

4.8.3 Problem with attempt 2

There are a few problems with the way attempt 2 was made, albeit it progressed further than attempt 1, without much assumption on the form of the infinite limit terms:

- 1. We do not understand what is the *error function* in this case, except from the fact that it is present in the integral table typically used for quantum mechanical system (basically a reference table).
- 2. We did not indict the physical interpretation of the solution by itself.
- 3. The Hermite polynomial and its terms are dubious, in the sense that we do not understand its nature in the fullest.

Appendix

4.8.4 Derivation of Schrödinger equation

We do not have enough rigour for a full realization of the Schrödinger equation. However, we can attempt and summarize the way in which it can be derived from classical mechanics concepts.

We consider the one-dimensional classical wave equation:

$$\frac{\partial^2 E}{\partial^2 x} - \frac{1}{c^2} \frac{\partial^2 E}{\partial^2 t} = 0 \tag{4.63}$$

This equation is satisfied by plane wave solution,

$$E(x,t) = E_0 e^{i(kx - \omega t)} \tag{4.64}$$

where $k=2\pi/\lambda$ and $\omega=2\pi\nu$ are the spatial and temporal frequencies, respectively. This then must satisfy the dispersion relation:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) E_0 e^{i(kx - \omega t)} = 0, \tag{4.65}$$

$$\left(-k^2 + \frac{\omega^2}{c^2}\right) E_0 e^{i(kx - \omega t)} = 0.$$
 (4.66)

Solving this for the wave vector, we arrive at the dispersion relation for light in free space:

$$k = \frac{\omega}{c} \tag{4.67}$$

or more familiarly, $\nu\lambda=c$, where c is the wave propagation speed. We recall that $\mathcal{E}=h\nu=\hbar\omega$, and $p=h/\lambda=\hbar k$. Rewrite this gives:

$$E(x,t) = E_0 e^{i/h(px - \mathcal{E}t)}$$

Substitute this to equation 2.5, we have:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right) E_0 e^{\frac{i}{\hbar}(px - \mathcal{E}t)} = 0,$$
(4.68)

$$-\frac{1}{\hbar^2} \left(p^2 - \frac{\mathcal{E}^2}{c^2} \right) E_0 e^{\frac{i}{\hbar} (px - \mathcal{E}t)} = 0.$$

$$\tag{4.69}$$

or $\mathcal{E} = p^2 c^2$. This is the relativistic total energy:

$$\mathcal{E}^2 = p^2 c^2 + m^2 c^4 \tag{4.70}$$

for a particle with zero rest mass. We know assume that frequency, energy and wavelength, and momentum are related in the same way for particles, as for photons (De Broglie). We consider a wave equation for non-zero rest mass particles. Call the wave equation Ψ . Since the above is heterogenous, we would then write:

$$0 = \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2}\right) \Psi e^{\frac{i}{\hbar}(px - \mathcal{E}t)}$$

$$0 = -\frac{1}{\hbar^2} \left(p^2 - \frac{\mathcal{E}^2}{c^2} + m^2 c^2\right) \Psi e^{\frac{i}{\hbar}(px - \mathcal{E}t)}.$$

$$(4.71)$$

Now, for the wavefunction Ψ , the energy density of the electrical field \mathbf{E} is realized by $|\mathbb{E}|^2$. The energy of an individual photon depends only on the frequency of light, $\epsilon = hf$, so $|\mathbb{E}|^2$ is proportional to the number of photons. By analogy, we demand that

$$\Psi(x,t) = \Psi_0(e^{i/h}(px - \mathcal{E}t)) \tag{4.72}$$

to be normalized to unit probability. Then, the probability that the particle is located somewhere in space, or

$$\int_{-\infty}^{\infty} \Psi^* \Psi \, dx = 1 \tag{4.73}$$

The existence of the plane waves, that is

$$\phi(r,t) \sim \exp\left(ik \cdot r - i\omega t\right)$$
 (4.74)

satisfying de Broglie and Einstein relations, implies the quantum interpretation of:

$$p \to -i\hbar \nabla, \quad E \to i\hbar \frac{\partial}{\partial t}$$
 (4.75)

For the relativistic energy-momentum equation, we get

$$E^2 = \mathbf{p}^2 c^2 + m^2 c^4 \tag{4.76}$$

which implies the Klein-Gordon equation:

$$-\hbar^2 \frac{\partial^2 \phi}{\partial t^2} = -\hbar^2 c^2 \nabla^2 \phi + m^2 c^4 \phi \tag{4.77}$$

Equation 4.71, removing the restriction on one dimension and rearranging them is similar to the Klein-Gordon equation for a free particle. Since it is relativistic, we ought to remove such aspect of it. We consider the approximate case of $\mathcal{E}^2 = (pc)^2 + m^2c^4$ by

$$\mathcal{E} \approx mc^2 \sqrt{1 + \frac{p^2}{m^2 c^2}} \approx mc^2 + \frac{p^2}{2m} = mc^2 + \mathcal{T}$$
 (4.78)

Klein-Gordon equation 4.8. Solution 47

This is the classial kinetic energy, for \mathcal{T} . We then rewrite Ψ as

$$\Psi(x,t) = \exp\left(-\frac{i}{\hbar}mc^2t\right)\Psi_0 \exp\left(\frac{i}{\hbar}(px - \mathcal{T}t)\right)$$
(4.79)

Assuming $mv \ll mc$, which means $p^2 \ll m^2c^2$. This means that

$$\exp\left(\frac{i}{\hbar}(px - \mathcal{T}t)\right) \in \left\{\exp\left(-\frac{i}{\hbar}mc^2t\right)\right\} \tag{4.80}$$

for little o notation, and in terms of the oscillation speed, which means the LHS is much slower. We then can write $\Psi = \exp{-i/\hbar(mc^2t)}\psi$, where $\psi = \Psi_0 \exp{i/\hbar(px - \mathcal{T}t)}$. Solving this for $\partial \Psi/\partial t$, we have:

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} mc^2 e^{-\frac{i}{\hbar} mc^2 t} \phi + e^{-\frac{i}{\hbar} mc^2 t} \frac{\partial \phi}{\partial t}$$
(4.81)

$$\frac{\partial^2 \Psi}{\partial t^2} = \left(-\frac{m^2 c^4}{\hbar^2} e^{-\frac{i}{\hbar} mc^2 t} \phi - \frac{2i}{\hbar} mc^2 e^{-\frac{i}{\hbar} mc^2 t} \frac{\partial \phi}{\partial t} \right) + e^{-\frac{i}{\hbar} mc^2 t} \frac{\partial^2 \phi}{\partial t^2}. \tag{4.82}$$

We discard the small terms. Using this approximation, we find that:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2im}{\hbar} \frac{\partial \psi}{\partial t} = 0 \tag{4.83}$$

which, rearranging a bit, will give the Schrödinger equation.

4.8.5 Bloch's theorem

Bloch's theorem is a central result for analysing semiconducting structure. For band structure in problems with periodic potential, it is important in such analysis, as well as the concept of periodic potentials in lattices.

A periodic potential appears because the ions are arranged with a periodicity of their Bravais lattice, given by the lattice vectors \mathbb{R}

$$U(\backslash + \mathbb{R}) = U(\backslash) \tag{4.84}$$

This potential enters into the Schrödinger equation as:

$$\hat{H}\psi = \left(-\frac{\hbar}{2m}\nabla^2 + U(\mathbf{r})\right)\psi = \epsilon\psi \tag{4.85}$$

The potential there is assumed to be spatially periodic, or V(x + a) = V(x). We assume the lattice goes on forever. The electrons are no longer free electrons, but are now called *Bloch electrons*.

From this, the Bloch's theorem states that:

Theorem 4.8.1 (Bloch's theorem). Theorem: The eigenstates ψ of the Hamitonian \hat{H} above can be chosen to have the form of a plane wave times a function with the periodicity of the Bravais lattice:

$$\psi_{nk}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{nk}(\mathbf{r})$$

where

$$u_{nk}(\mathbf{r} + \mathbf{R}) = u_{nk}(\mathbf{r})$$

The quantum number n is called the ${\it band index}$ and takes numbers $n=1,2,3,\ldots$

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List of problems in theoretical mechanics

Introduction

There are not a lot of things to say about this section others than it being served to record a lot of the problems I encountered in the course of theoretical mechanics. It being here is not just cosmetic, somehow, but certainly for logging before the final test (perhaps).

Lagrangian mechanics

Single pendulum

The single pendulum has one single generalized coordinate ϕ . This is illustrated as the following figures: Then, the kinetic energy is as usual,

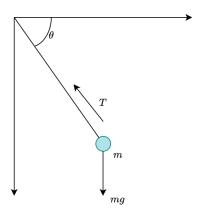


Figure 1: Diagram of a single pendulum with a single mass m and a rod of length ℓ connecting it.

$$T = \sum_{a} \frac{m_a v_a^2}{2} = \frac{m}{2} (\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$
 (4.86)

We have for the object m in the coordinate:

$$x_m = \ell \sin(\phi), \quad y_m = \ell \cos(\phi), \quad z = 0$$
 (4.87)

Hence, substitute into T we gain:

$$T = \frac{m}{2} \left[(\ell \sin \phi)^{2} + (\ell \cos \phi)^{2} \right]$$

$$= \frac{m}{2} \left[\ell^{2} \dot{\phi}^{2} \cos^{2} \phi + \ell^{2} \dot{\phi}^{2} \sin^{2} \phi \right]$$

$$= \frac{m\ell^{2} \dot{\phi}^{2}}{2}$$

$$(4.88)$$

Choose the origin at the surface A downward from the top, then, $U=mgh=-mg\ell\cos\phi$. The Lagrangian is then:

$$\mathcal{L} = T - U = \frac{m\ell^2 \dot{\phi}^2}{2} + mg\ell \cos \phi \tag{4.89}$$

To derive this for the Euler-Lagrange equation, we first give two arguments:

$$\frac{\partial \mathcal{L}}{\partial \phi} = -mg\ell \sin \phi, \quad \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = m\ell^2 \dot{\phi}$$
 (4.90)

Then, the Euler-Lagrange reads:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \tag{4.91}$$

$$\frac{d}{dt}(m\ell^2\dot{\phi}) + mgl\sin\phi = 0$$

$$m\ell^2\ddot{\phi} + mg\ell\sin\phi = 0$$
(4.92)
(4.93)

$$m\ell^2\ddot{\phi} + mg\ell\sin\phi = 0\tag{4.93}$$

Double pendulum

For the double pendulum, there are two generalized coordinates ϕ_1, ϕ_2 . Thus the function

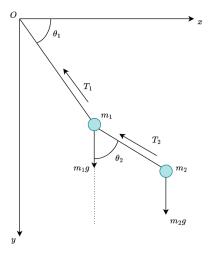


Figure 2: Diagram of a double pendulum with two masses: m_1 and m_2 , with their respective ℓ_1 connecting the origin to m_1 , and ℓ_2 connecting m_1 to m_2 .

would then be counted by the generalized velocity $\dot{\phi}_1, \dot{\phi}_2$. For two masses m_1, m_2 , we have:

$$\begin{cases} x_1 = l_1 \sin \phi_1 \\ y_1 = l_1 \cos \phi_1 \end{cases}, \begin{cases} x_1 = x_1 + l_2 \sin \phi_2 \\ y_1 = y_1 + l_2 \cos \phi_2 \end{cases}, \tag{4.94}$$

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Which gives:

$$\begin{cases} \dot{x}_1 = l_1 \dot{\phi}_1 \cos \phi_1 \\ \dot{y}_1 = -l_1 \dot{\phi}_1 \sin \phi_1 \end{cases}, \begin{cases} \dot{x}_2 = l_1 \dot{\phi}_1 \cos \phi_1 + l_2 \dot{\phi}_2 \cos \phi_2 \\ \dot{y}_2 = -l_1 \dot{\phi}_1 \sin \phi_1 - l_2 \dot{\phi}_2 \sin \phi_2 \end{cases}$$
(4.95)

The kinetic energy is formulated such that:

$$T = \frac{m_1 v_1^2}{2} + \frac{m_2 v_2^2}{2} \tag{4.96}$$

$$=\frac{m_1}{2}(\dot{x}_1^2+\dot{y}_1^2)+\frac{m_2}{2}(\dot{x}_2^2+\dot{y}_2^2) \tag{4.97}$$

$$= \frac{m_1}{2} \left(l_1^2 \dot{\phi}_1^2 \cos^2 \phi_1 + l_2^2 \dot{\phi}_2^2 \cos^2 \phi_2 \right) + \frac{m_2}{2} \left[\left(l_1 \dot{\phi}_1 \cos \phi_1 + l_2 \dot{\phi}_2 \cos \phi_2 \right)^2 \right]$$
(4.98)

$$+\frac{m_1}{2} \left[\left(l_1 \dot{\phi}_1 \sin \phi_1 + l_2 \dot{\phi}_2 \sin \phi_2 \right)^2 \right] \tag{4.99}$$

$$= \frac{m_1}{2} l_1^2 \dot{\phi}_1^2 + \frac{m_2}{2} \left[l_1^2 \dot{\phi}_1^2 \cos^2 \phi_1 + 2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \cos \phi_1 \cos \phi_2 + l_2^2 \dot{\phi}_2^2 \cos^2 \phi_2 \right]$$
(4.100)

$$+\frac{m_2}{2}\left[l_1^2\dot{\phi}_1^2\sin^2\phi_1 + 2\,l_1l_2\,\dot{\phi}_1\dot{\phi}_2\,\sin\phi_1\sin\phi_2 + l_2^2\dot{\phi}_2^2\sin^2\phi_2\right] \tag{4.101}$$

$$= \frac{m_1}{2} l_1^2 \dot{\phi}_1^2 + \frac{m_2}{2} \left(l_1^2 \dot{\phi}_1^2 + 2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \cos(\phi_1 - \phi_2) + l_2^2 \dot{\phi}_2^2 \right)$$
(4.102)

$$= \frac{1}{2}(m_1 + m_2) l_1^2 \dot{\phi}_1^2 + m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \cos(\phi_1 - \phi_2) + \frac{1}{2} m_2 l_2^2 \dot{\phi}_2^2.$$
 (4.103)

The above derivation uses specifically two elementary trigonometric relations:

$$\cos a - b = \cos a \cos b + \sin a \sin b, \quad \sin^2 a + \cos^2 a = 1$$
 (4.104)

Choose the origin at A of the hanging point such that mgy = 0. The potential energy is then:

$$U = -m_1 g l_1 \cos \phi_1 - m_2 g [l_1 \cos \phi_1 + l_2 \cos \phi_2]$$
(4.105)

The Lagrangian is then expressed as:

$$L = T - V$$

$$= \frac{1}{2} (m_1 + m_2) l_1^2 \dot{\phi}_1^2 + m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \cos(\phi_1 - \phi_2) + \frac{1}{2} m_2 l_2^2 \dot{\phi}_2^2$$

$$+ m_1 q l_1 \cos \phi_1 + m_2 q [l_1 \cos \phi_1 + l_2 \cos \phi_2]$$

$$(4.106)$$

Now, to obtain the Euler-Lagrange form, we then have to derive $\partial \mathcal{L}/\partial \phi_1$, $\partial \mathcal{L}/\partial \phi_2$ and their respective generalized velocity. This gives the following:

$$\frac{\partial L}{\partial \dot{\phi}_1} = (m_1 + m_2) l_1^2 \dot{\phi}_1 + m_2 l_1 l_2 \dot{\phi}_2 \cos(\phi_1 - \phi_2), \tag{4.107}$$

$$\frac{\partial L}{\partial \dot{\phi}_2} = m_2 \, l_2^2 \, \dot{\phi}_2 + m_2 \, l_1 \, l_2 \, \dot{\phi}_1 \, \cos(\phi_1 - \phi_2), \tag{4.108}$$

$$\frac{\partial L}{\partial \phi_1} = -m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - (m_1 + m_2) g l_1 \sin \phi_1, \tag{4.109}$$

$$\frac{\partial L}{\partial \phi_2} = + m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - m_2 g l_2 \sin \phi_2. \tag{4.110}$$

We can then substitute this back to the Euler-Lagrange equation to give the following set of two equations' solutions:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}_1} \right) - \frac{\partial \mathcal{L}}{\partial \phi_1} = 0, \quad \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}_2} \right) - \frac{\partial \mathcal{L}}{\partial \phi_2} = 0 \tag{4.111}$$

That is,

$$(m_1 + m_2)l_1^2\phi_1 + m_2l_1l_2(\ddot{\phi}\cos(\phi_1 - \phi_2)) + \phi_2[-\sin(\phi_1 - \phi_2)(\dot{\phi}_1 - \dot{\phi}_2)] = 0$$

$$-m_2gl_2\sin\phi_2 + m_2\dot{\phi}_2\dot{\phi}_1l_2l_1\sin(\phi_1 - \phi_2) = 0$$
(4.113)

Single pendulum with moving support

The setting looks kind of like this, with one single mass m_1 and a moving support point on the horizontal side:

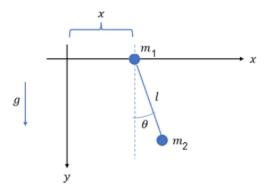


Figure 3: A pendulum system with moving horizontal support.

The number of degree of freedom is hence 2, for x, ϕ as the angle (obviously) thus their generalized velocity $\dot{x}, \dot{\phi}$. Then, we have:

$$\begin{cases} x_m = x + l\sin\phi \\ y_m = l\cos\phi \end{cases} \tag{4.114}$$

Standard xyz indicts the following generalized system:

$$\begin{cases} x_m = x + l \sin \phi \\ y_m = l \cos \phi \\ z_m = 0 \end{cases} \Rightarrow \begin{cases} \dot{x}_m = \dot{x} + l \dot{\phi} \cos \phi \\ \dot{y}_m = -l \dot{\phi} \sin \phi \\ \dot{z}_m = 0 \end{cases}$$
(4.115)

The kinetic energy T of the Lagrangian is then as:

$$T = \frac{m}{2} \left[(x' + l\dot{\phi}\cos\phi)^2 + (l\dot{\phi}\sin\phi)^2 \right]$$

$$= \frac{m}{2} \left[\dot{x}^2 + 2\dot{x}l\dot{\phi}\cos\phi + l^2\dot{\phi}^2\cos^2\phi + l^2\dot{\phi}^2\sin^2\phi \right]$$

$$= \frac{m}{2} \left(\dot{x}^2 + 2\dot{x}l\dot{\phi}\cos\phi + l^2\dot{\phi}^2 \right)$$
(4.116)

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Choose the origin (as for potential energy) at y=0, then $U=-mgl\cos\phi$. The Lagrangian then can be written as:

$$\mathcal{L} = T - U = \frac{m}{2} \left(\dot{x}^2 + 2\dot{x}l\dot{\phi}\cos\phi + l^2\dot{\phi}^2 \right) + mgl\cos\phi \tag{4.117}$$

The Euler-Lagrange equation then consists of again, four terms:

$$\frac{\partial \mathcal{L}}{\partial x} = 0, \qquad \frac{\partial \mathcal{L}}{\partial \dot{x}} = m \, \dot{x} + m \, l \, \dot{\phi} \cos \phi,
\frac{\partial \mathcal{L}}{\partial \phi} = -m \, l \, \dot{x} \, \dot{\phi} \sin \phi - m \, g \, l \sin \phi, \qquad \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = m \, l \, \dot{x} \cos \phi + m \, l^2 \, \dot{\phi}.$$
(4.118)

The two Euler-Lagrange equations can be derived naturally by application. The first one for ϕ :

$$\frac{d}{dt}\left(m\,l\,\dot{x}\,\cos\phi + m\,l^2\,\dot{\phi}\right) - \left[-\,m\,l\,\dot{x}\,\dot{\phi}\,\sin\phi - m\,g\,l\,\sin\phi\right] = 0 \tag{4.119}$$

$$ml\ddot{x}\cos\phi + ml^2\ddot{\phi} + mgl\sin\phi = 0 \tag{4.120}$$

And the second one for x (which is much simpler):

$$\frac{d}{dt}\left(m\,\dot{x} + m\,l\,\dot{\phi}\,\cos\phi\right) = 0\tag{4.121}$$

$$m\ddot{x} + ml\ddot{\phi}\cos\phi + ml\dot{\phi}^2\sin\phi = 0 \tag{4.122}$$

Pendulum with rotating support

It is better illustrated of an illustration. This time, we have a single pendulum of mass m and rod length l, and a uniform circular motion of a ring with origin O fixed. with this kind of problem, usually there are two configurations:

- 1. The point of potential energy is perpendicular, that is, t = 0, A = Oy for particular point of connection A between the rotating support and the pendulum.
- 2. The point of potential energy is horizontal, that is, t = 0, A = Ox.

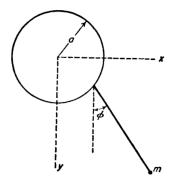


Figure 4: Illustration of a pendulum of mass m and length l, with support moving uniformly on a circular ring of radius r.

We will resolve the first case first. The other case will follow shortly, after all. The generalized coordinate is just one, since A is fixed of radius r and time evolution t. Then, we have ϕ , $\dot{\phi}$ as

the coordinate and its velocity. Then,

$$\begin{cases} x_A = R\cos\omega t - \frac{\pi}{2} \\ y_A = -R\sin\omega t - \frac{\pi}{2} \end{cases} \Leftrightarrow \begin{cases} x_A = R\sin\omega t \\ y_A = R\cos\omega t \end{cases}$$
 (4.123)

Hence, we have:

$$\begin{cases} x_m = R\sin(\omega t) + l\sin\phi \\ y_m = R\cos(\omega t) + l\cos\phi \end{cases}$$
(4.124)

and hence the velocity is:

$$\dot{x}_m = R\omega\cos\omega t + l\dot{\phi}\cos\phi\dot{y}_m = -R\omega\sin\omega t - l\dot{\phi}\sin\phi \tag{4.125}$$

The kinetic energy T is hence:

$$T = \frac{m}{2}(\dot{x}^2 + \dot{y}^2)$$

$$T = \frac{m}{2}\left(\left[R\omega\cos\omega t + l\dot{\phi}\cos\phi\right]^2 - \left[-R\omega\sin\omega t - l\dot{\phi}\sin\phi\right]^2\right)$$

$$\frac{2}{m}T = \left[R\omega\cos\omega t\right]^2 + 2l\dot{\phi}\sin\phi R\omega\cos\omega t + \left[l\dot{\phi}\sin\phi\right]^2$$

$$-\left[\left(-R\omega\sin\omega t\right)^2 + 2R\omega\sin(\omega t)l\dot{\phi}\sin\phi + \left(l\dot{\phi}\sin\phi\right)^2\right]$$

$$= (R\omega)^2 + (l\dot{\phi})^2 + 2R\omega l\dot{\phi}(\cos\omega t\cos\phi + \sin\omega t\sin\phi)$$

$$= R^2\omega^2 + l^2\dot{\phi}^2 + 2R\omega l\dot{\phi}\cos(\omega t - \phi)$$

$$(4.126)$$

The potential energy at Oy is hence $U = -mgh = -mg[R\cos\omega t + l\cos\omega t]$. Hence, the Lagrangian is thus:

$$\mathcal{L} = T - U = R^2 \omega^2 + l^2 \dot{\phi}^2 + 2R\omega l \dot{\phi} \cos(\omega t - \phi) + mg \left[R \cos \omega t + l \cos \omega t \right]$$
 (4.127)

The Euler-Lagrange equation is calculated accordingly, and the second case is also derived in the same way, albeit without $\pi/2$. For such case, we have:

$$\begin{pmatrix} x_A \\ y_A \end{pmatrix} = \begin{pmatrix} R\cos(\omega t) \\ -R\sin(\omega t) \end{pmatrix} = \begin{pmatrix} R\cos(\omega t) \\ R\sin(-\omega t) \end{pmatrix}$$
 (4.128)

That is, for the pendulum,

$$\begin{pmatrix} x_m \\ y_m \end{pmatrix} = \begin{pmatrix} R\cos(\omega t) \\ R\sin(-\omega t) \end{pmatrix} + \begin{pmatrix} l\sin\phi \\ l\cos\phi \end{pmatrix}$$
 (4.129)

At this point, we somewhat remark a small point in this derivation. Here, even though we choose $-R\sin{(\omega t)}$, why we do not have $l\sin{\phi}$ and the cosine one do the same? The reason is fairly simple – we kinda flipped the whole thing downward. Now, this is perhaps troublesome, since $l\sin{\phi}$ is alright, but $\sin{\omega t}$ is negative in the third and fourth quadrant, to reflect the negative sections. And if you question more about the angle reversion and clockwise rotation, well, just like me, look up quadrant and even-odd properties of them. Now, this means:

$$\begin{pmatrix} \dot{x}_m \\ \dot{y}_m \end{pmatrix} = \begin{pmatrix} -R\sin(\omega t) + l\dot{\phi}\cos\phi \\ R\cos(\omega t) - l\dot{\phi}\sin\phi \end{pmatrix}$$
 (4.130)

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The kinetic energy is hence:

$$T = \frac{m}{2} \left(\dot{x}^2 + \dot{y}^2 \right)$$

$$= \frac{m}{2} \left[\left(-R \sin(\omega t) + l \dot{\phi} \cos \phi \right)^2 + \left(R \cos(\omega t) - l \dot{\phi} \sin \phi \right)^2 \right]$$

$$= \frac{m}{2} \left[R^2 \sin^2(\omega t) + l^2 \dot{\phi}^2 \cos^2 \phi - 2R l \dot{\phi} \sin(\omega t) \cos \phi$$

$$+ R^2 \cos^2(\omega t) + l^2 \dot{\phi}^2 \sin^2 \phi - 2R l \dot{\phi} \cos(\omega t) \sin \phi \right]$$

$$= \frac{m}{2} \left[R^2 \left(\sin^2(\omega t) + \cos^2(\omega t) \right) + l^2 \dot{\phi}^2 \left(\cos^2 \phi + \sin^2 \phi \right)$$

$$- 2R l \dot{\phi} \left(\sin(\omega t) \cos \phi + \cos(\omega t) \sin \phi \right) \right]$$

$$= \frac{m}{2} \left[R^2 + l^2 \dot{\phi}^2 - 2R l \dot{\phi} \sin(\omega t + \phi) \right].$$
(4.131)

Now, the potential energy is simply $U = -mgh = -[R\sin{(-\omega t)} + l\cos{\phi}]$. The obtained Lagrangian is hence:

$$\mathcal{L} = T - U = \frac{m}{2} \left[R^2 + l^2 \dot{\phi}^2 - 2R l \dot{\phi} \sin(\omega t + \phi) \right] + \left[R \sin(-\omega t) + l \cos \phi \right]$$
 (4.132)

The Euler-Lagrange proceed as always.

Pendulum with oscillating support

Now, we remember the horizontal support case, yeah? Now, we also put a constraint named $x=a\cos\omega t$ on it. Then, the generalized coordinate count reduces by 1, since x is now prescribed; so ϕ , $\dot{\phi}$ is the only pair. We then have:

$$\begin{pmatrix} x_m \\ y_m \end{pmatrix} = \begin{pmatrix} x + l\sin\phi \\ l\cos\phi \end{pmatrix} = \begin{pmatrix} a\cos\omega t + l\sin\phi \\ l\cos\phi \end{pmatrix}$$
(4.133)

and hence,

$$\begin{pmatrix} \dot{x}_m \\ \dot{y}_m \end{pmatrix} = \begin{pmatrix} -a\omega\sin\omega t + l\dot{\phi}\cos\phi \\ -l\dot{\phi}\sin\phi \end{pmatrix}$$
 (4.134)

The kinetic energy T is then:

$$T = \frac{m}{2} \left(\dot{x}^2 + \dot{y}^2 \right)$$

$$= \frac{m}{2} \left[\left(\dot{x} + l \,\dot{\phi} \cos \phi \right)^2 + \left(-l \,\dot{\phi} \sin \phi \right)^2 \right]$$

$$= \frac{m}{2} \left[\left(-a \,\omega \sin(\omega t) + l \,\dot{\phi} \cos \phi \right)^2 + \left(-l \,\dot{\phi} \sin \phi \right)^2 \right]$$

$$= \frac{m}{2} \left[a^2 \,\omega^2 \sin^2(\omega t) - 2 \,a \,\omega \,l \,\dot{\phi} \sin(\omega t) \cos \phi + l^2 \,\dot{\phi}^2 \cos^2 \phi + l^2 \,\dot{\phi}^2 \sin^2 \phi \right]$$

$$= \frac{m}{2} \left[a^2 \,\omega^2 \sin^2(\omega t) - 2 \,a \,\omega \,l \,\dot{\phi} \sin(\omega t) \cos \phi + l^2 \,\dot{\phi}^2 \left(\cos^2 \phi + \sin^2 \phi \right) \right]$$

$$= \frac{m}{2} \left[a^2 \,\omega^2 \sin^2(\omega t) + l^2 \,\dot{\phi}^2 - 2 \,a \,\omega \,l \,\dot{\phi} \sin(\omega t) \cos \phi \right].$$
(4.135)

The kinetic energy for potential origin at y=0 is thus $U=-mgh=-mgl\cos\phi$. The Lagrangian is hence:

$$\mathcal{L} = T - U = \frac{m}{2} \left[a^2 \omega^2 \sin^2(\omega t) + l^2 \dot{\phi}^2 - 2 a \omega l \dot{\phi} \sin(\omega t) \cos \phi \right] + mgl \cos \phi \qquad (4.136)$$

The Euler-Lagrange equation would be

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \tag{4.137}$$

$$ml^2\dot{\phi} - mla\omega^2\cos\omega t\cos\phi = -mgl\sin\phi \tag{4.138}$$

Now, in the case where the oscillation is in the **vertical** y **direction**, we have the similar case. Slightly different, nevertheless.

$$\begin{pmatrix} x_m \\ y_m \end{pmatrix} = \begin{pmatrix} l \sin \phi \\ l \cos \phi + a \cos \omega t \end{pmatrix}$$
 (4.139)

The derivative is then:

$$\begin{pmatrix} \dot{x}_m \\ \dot{y}_m \end{pmatrix} = \begin{pmatrix} i\dot{\phi}\cos\phi \\ -i\dot{\phi}\sin\phi - a\omega\sin\omega t \end{pmatrix} \tag{4.140}$$

The kinetic energy is then:

$$T = \frac{m}{2} \left[\left(l\dot{\phi}\cos\phi \right)^2 + \left(-l\dot{\phi}\sin\phi - a\omega\sin\omega t \right)^2 \right]$$

$$= \frac{m}{2} \left[l^2\dot{\phi}^2\cos^2\phi + l^2\dot{\phi}^2\sin^2\phi + 2l\dot{\phi}\sin\phi a\omega\sin\omega t + a^2\omega^2\sin^2\omega t \right]$$

$$= \frac{m}{2} \left[l^2\dot{\phi}^2 + 2al\omega\dot{\phi}\sin\phi\sin(\omega t) + a^2\omega^2\sin^2(\omega t) \right].$$
(4.141)

Set the potential origin at y=0, then $U=-mgh=-mg(l\cos\phi+a\cos\omega t)$. The Lagrangian is then

$$\mathcal{L} = T - U = \frac{m}{2} \left[l^2 \dot{\phi}^2 + 2al\omega \dot{\phi} \sin \phi \sin (\omega t) + a^2 \omega^2 \sin^2 (\omega t) \right] + mg(l\cos \phi + a\cos \omega t)$$
(4.142)

The derivation of single generalized coordinate Euler-Lagrange equation follows as usual.

Constrained 1D grapple motion

The situation is more easily presented with an illustration. Partially because I don't know what is this called as, so pretty lame. There is only one generalized coordinate ϕ . The positional equation is then

$$\begin{pmatrix} x_m \\ y_m \end{pmatrix} = \begin{pmatrix} 2l\cos\phi \\ 0 \end{pmatrix}$$
 (4.143)

Hence, the velocity differential is as:

$$\begin{pmatrix} \dot{x}_m \\ \dot{y}_m \end{pmatrix} = \begin{pmatrix} -2l\dot{\phi}\sin\phi \\ 0 \end{pmatrix} \tag{4.144}$$

The kinetic energy is simple,

$$T = \frac{m}{2} \left(4l^2 \dot{\phi}^2 \sin^2 \phi \right) = 2ml^2 \dot{\phi}^2 \sin^2 \phi \tag{4.145}$$

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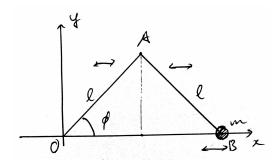


Figure 5: Constrained 1D grapple motion of the isosceles triangle of l on both side, mass m movement restricted to the Ox plane.

Choose the potential origin at the plane y=0, then U=mgy=0. The Lagrangian is simple:

$$\mathcal{L} = T - U = 2ml^2 \dot{\phi}^2 \sin^2 \phi \tag{4.146}$$

The Lagrangian is simpler

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}} \right) - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \tag{4.147}$$

$$\frac{d}{dt} \left(4 m l^2 \dot{\phi} \sin^2 \phi \right) - 4 m l^2 \dot{\phi}^2 \sin \phi \cos \phi = 0$$
 (4.148)

$$4 m l^{2} \left(\ddot{\phi} \sin^{2} \phi + \dot{\phi} \frac{d}{dt} (\sin^{2} \phi) \right) - 4 m l^{2} \dot{\phi}^{2} \sin \phi \cos \phi = 0$$
 (4.149)

$$4 m l^{2} \left(\ddot{\phi} \sin^{2} \phi + \dot{\phi} \left(2 \sin \phi \cos \phi \dot{\phi} \right) \right) - 4 m l^{2} \dot{\phi}^{2} \sin \phi \cos \phi = 0$$
 (4.150)

$$4 m l^2 \left(\ddot{\phi} \sin^2 \phi + 2 \dot{\phi}^2 \sin \phi \cos \phi \right) - 4 m l^2 \dot{\phi}^2 \sin \phi \cos \phi = 0$$
 (4.151)

$$4 m l^2 \left(\ddot{\phi} \sin^2 \phi + \dot{\phi}^2 \sin \phi \cos \phi \right) = 0$$
 (4.152)

$$\ddot{\phi}\sin^2\phi + \dot{\phi}^2\sin\phi\cos\phi = 0 \tag{4.153}$$

Connected 3-mass springs

The situation is described by the following illustration. Here, note that the notation Δx is there for completeness and customary, though usually we would just refer to such distance as the stretch distance calculated of the potential energy from the restoring forces. Then, the degree of freedom is 3, x_1, x_2, x_3 and $\dot{x}_1, \dot{x}_2, \dot{x}_3$ as their generalized coordinate. As such, the kinetic energy is:

$$T = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 \tag{4.154}$$

Because there exists no gravitational potential, hence the potential energy is in the spring itself, that is,

$$U = \frac{1}{2}k_1x_1^2 + \frac{1}{2}k_2(x_2 - x_1)^2 + \frac{1}{2}k_3(x_3 - x_2)^2$$
(4.155)

The Lagrangian is then:

$$\mathcal{L} = T - U = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \left(\frac{1}{2}k_1x_1^2 + \frac{1}{2}k_2(x_2 - x_1)^2 + \frac{1}{2}k_3(x_3 - x_2)^2\right)$$
(4.156)

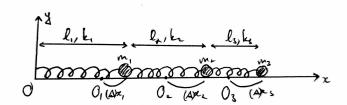


Figure 6: Constrained one-dimensional motion of three masses m_1, m_2, m_3 connected to each others of three springs l_1, l_2, l_3 (connected to also the origin) for spring constant k_1, k_2, k_3 , and equilibrium points O_1, O_2, O_3 .

Solving this for the Euler-Lagrange equation gives six component equations:

$$\frac{\partial \mathcal{L}}{\partial \dot{x}_1} = m_1 \, \dot{x}_1,\tag{4.157}$$

$$\frac{\partial \mathcal{L}}{\partial \dot{x}_2} = m_2 \, \dot{x}_2,\tag{4.158}$$

$$\frac{\partial \mathcal{L}}{\partial \dot{x}_3} = m_3 \, \dot{x}_3,\tag{4.159}$$

$$\frac{\partial \mathcal{L}}{\partial x_1} = -k_1 x_1 + k_2 (x_2 - x_1), \tag{4.160}$$

$$\frac{\partial \mathcal{L}}{\partial x_2} = -k_2 (x_2 - x_1) + k_3 (x_3 - x_2), \tag{4.161}$$

$$\frac{\partial \mathcal{L}}{\partial x_3} = -k_3 \left(x_3 - x_2 \right). \tag{4.162}$$

Applying this to all Euler-Lagrange equations:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}_1} \right) - \frac{\partial \mathcal{L}}{\partial x_1} = 0 \tag{4.163}$$

$$m_1 \ddot{x}_1 - (-k_1 x_1 + k_2 (x_2 - x_1)) = 0$$
 (4.164)

$$m_1 \ddot{x}_1 + k_1 x_1 - k_2 (x_2 - x_1) = 0$$
 (4.165)

$$m_1 \ddot{x}_1 + (k_1 + k_2) x_1 - k_2 x_2 = 0$$
 (4.166)

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}_2} \right) - \frac{\partial \mathcal{L}}{\partial x_2} = 0 \tag{4.167}$$

$$m_2 \ddot{x}_2 - (-k_2(x_2 - x_1) + k_3(x_3 - x_2)) = 0$$
 (4.168)

$$m_2 \ddot{x}_2 + k_2 (x_2 - x_1) - k_3 (x_3 - x_2) = 0$$
 (4.169)

$$m_2 \ddot{x}_2 + (k_2 + k_3) x_2 - k_2 x_1 - k_3 x_3 = 0$$
 (4.170)

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{x}_3} \right) - \frac{\partial \mathcal{L}}{\partial x_3} = 0 \tag{4.171}$$

$$m_3 \ddot{x}_3 - (-k_3 (x_3 - x_2)) = 0$$
 (4.172)

$$m_3 \ddot{x}_3 + k_3 (x_3 - x_2) = 0$$
 (4.173)

$$m_3 \ddot{x}_3 + k_3 x_3 - k_3 x_2 = 0 (4.174)$$

Conservation laws in Lagrangian terms

In this section, there is only two exercises of interest. However, to solve them quicker, we have some tricks. Or rather one but very effective one. The momentum M in a Lagrangian system, aside from its conservation law (not of our interest) is taken in the form:

$$M = \left[\vec{r} \times \vec{P} \right] = m \left[\vec{r} \times \vec{v} \right] \tag{4.175}$$

The product is calculated in a rather easy fashion as:

$$\vec{r} \times \vec{v} = \det \begin{bmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ \dot{x} & \dot{y} & \dot{z} \end{bmatrix}$$

$$= \hat{x} (y\dot{z} - z\dot{y}) + \hat{y} (\dot{x}z - \dot{z}x) + \hat{z} (x\dot{y} - y\dot{x})$$
(4.176)

Then, the momentum is thus as followed:

$$\begin{pmatrix}
M_x \\
M_y \\
M_z
\end{pmatrix} = \begin{pmatrix}
m (y\dot{z} - z\dot{y}) \\
m (\dot{x}z - \dot{z}x) \\
m (x\dot{y} - y\dot{x})
\end{pmatrix}$$
(4.177)

such that we have $M^2=M_x^2+M_y^2+M_z^2$. We then can further use this in analysing and solving momenta for spherical and cylindrical coordinates.

Cylindrical coordinates

$$x = r \cos \phi, \qquad \dot{x} = \dot{r} \cos \phi - r \dot{\phi} \sin \phi,$$

$$y = r \sin \phi, \qquad \dot{y} = \dot{r} \sin \phi + r \dot{\phi} \cos \phi,$$

$$z = z, \qquad \dot{z} = \dot{z},$$
(4.178)

$$M_{x} = m(y \dot{z} - z \dot{y}) = m \left(r \sin \phi \dot{z} - z (\dot{r} \sin \phi + r \dot{\phi} \cos \phi) \right),$$

$$M_{y} = m(z \dot{x} - x \dot{z}) = m \left(z (\dot{r} \cos \phi - r \dot{\phi} \sin \phi) - r \cos \phi \dot{z} \right),$$

$$M_{z} = m(x \dot{y} - y \dot{x}) = m r^{2} \dot{\phi}.$$

$$(4.179)$$

Spherical coordinates

$$x = r \sin \theta \cos \phi, \qquad \dot{x} = \dot{r} \sin \theta \cos \phi + r \dot{\theta} \cos \theta \cos \phi - r \dot{\phi} \sin \theta \sin \phi,$$

$$y = r \sin \theta \sin \phi, \qquad \dot{y} = \dot{r} \sin \theta \sin \phi + r \dot{\theta} \cos \theta \sin \phi + r \dot{\phi} \sin \theta \cos \phi,$$

$$z = r \cos \theta, \qquad \dot{z} = \dot{r} \cos \theta - r \dot{\theta} \sin \theta.$$
(4.180)

$$M_{x} = m(y \dot{z} - z \dot{y}) = -m r^{2} \left(\sin \phi \dot{\theta} + \sin \theta \cos \phi \cos \phi \dot{\phi} \right),$$

$$M_{y} = m(z \dot{x} - x \dot{z}) = m r^{2} \left(\cos \phi \dot{\theta} - \sin \theta \cos \theta \sin \phi \dot{\phi} \right),$$

$$M_{z} = m(x \dot{y} - y \dot{x}) = m r^{2} \sin^{2} \theta \dot{\phi}.$$

$$(4.181)$$

Finding momenta from Lagrangian

Here, we illustrate the problem of finding the momenta from a given Lagrangian equation. We have the Lagrangian of the form:

$$\mathcal{L} = \frac{1}{2}m(\alpha^2 + \beta^2)(\dot{\alpha}^2 + \dot{\beta}^2) + \frac{1}{2}m\alpha^2\beta^2\dot{\gamma}^2$$
 (4.182)

To find the momenta of this Lagrangian, simply take the partial derivative w.r.t. to each individual generalized velocity:

$$p_{\alpha} = \frac{\partial \mathcal{L}}{\partial \dot{\alpha}} = m(\alpha^2 + \beta^2)\dot{\alpha}$$
$$p_{\beta} = \frac{\partial \mathcal{L}}{\partial \dot{\beta}} = m(\alpha^2 + \beta^2)\dot{\beta}$$
$$p_{\gamma} = \frac{\partial \mathcal{L}}{\partial \dot{\gamma}} = m\alpha^2\beta^2\dot{\gamma}$$

Small oscillations

In this occasion, for the fourth section, the main focus is quite simple. Recall that to solve for small oscillations, means to fix and analyse the following equation:

$$\ddot{x} + \omega x = \frac{F(t)}{m} \tag{4.183}$$

The general solution of this equation is of the form $x = x_0 + x_1$, where x_0 is the solution for the homogeneous equation

$$\ddot{x} + \omega^2 x = 0 \tag{4.184}$$

and x_1 is the special solution for equation 4.183. If we try to solve for x_0 , we should have x_0 of the general form as

$$x_0 = C_1 \cos \omega t + C_2 \sin \omega t = a \cos \omega t + \phi \tag{4.185}$$

for

$$a = \sqrt{C_1^2 + C_2^2}, \quad \phi = \arctan C_2/C_1$$
 (4.186)

Now, for x_1 , the situation is a bit more convoluted. Here, we have that if the force F(t) is of the form:

$$F(t) = a_n t^n + a_{n-1} t^{n-1} + \dots + a_0 t^0$$
(4.187)

then x_1 would be equal to $b_nt^n+\cdots+b_0t^0$. To find the coefficient, simply substitute them in, and find each of the coefficient. The process can be tedious, however. The second case is if the force for F(t) is of the form $Ae^{\pm \alpha t}$, then $x_1=Be^{\pm \alpha t}$ and is solved for B accordingly. Let's take an example for $2t^2+5$. For this, then

$$\ddot{x} + \omega^2 x = \frac{2t^2 + 5}{m} \tag{4.188}$$

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The standard solution is $x = x_0 + x_1$. Then, $x_1 = at^2 + bt + c$ since F(t) is second order polynomial. Solving this for *x*:

$$\frac{d^2}{dt^2}(at^2 + bt + c) + \omega^2(at^2 + bt + c) = \frac{2t^2 + 5}{m}$$
(4.189)

$$a + \omega^2(at^2 + bt + c) = \frac{2t^2 + 5}{m}$$
(4.190)

$$\omega^2 a t^2 + \omega^2 b t + \omega^2 a c = \frac{2}{m} t^2 + \frac{5}{m}$$
 (4.191)

(4.192)

This gives

$$a = \frac{2}{m\omega^2}, \quad b = 0, \quad c = \frac{5}{m\omega^2}$$
 (4.193)

The solution for the standard solution would then be

$$x = C_1 \cos \omega t + C_2 \sin \omega t + \frac{2}{m\omega^2} t^2 + \frac{5}{m\omega^2}$$
 (4.194)

If we want to solve for C_1, C_2 , first we can get the derivative of x, that is

$$\dot{x} = -C_1 \omega \sin \omega t + C_2 \omega \cos \omega t + \frac{4t}{m\omega^2}$$
(4.195)

Then, use the case t=0. Then, either x=0 or x'=0. Substitute this into both equations for t = 0, then:

$$C_1 = -\frac{5}{m_{\rm c}r^2}, C_2 = -\frac{4t}{m_{\rm c}r^2}$$
 (4.196)

The solution is then:

$$x = -\frac{5}{m\omega^2}\cos\omega t - \frac{4t}{m\omega^2}\sin\omega t + \frac{2}{m\omega^2}t^2 + \frac{5}{m\omega^2}$$
 (4.197)

The same thing can be done with $Ae^{\pm \alpha t}$.

Problems

Setting 4.8.1. Determine the equation of motion for the following applied force for the equation $\ddot{x} + \omega^2 x =$ F(t)/m:

- 1. F(t) = 3.
- 2. F(t) = 2t.
- 3. F(t) = 3t + 1.

- 5. F(t) = 3t + 1. 4. $F(t) = 2t^2 + 5$. 5. $F(t) = at^2$. 6. $F(t) = 2t^2 + t$. 7. $F(t) = 3e^{2t}$.
- 8. $F(t) = 2e^{-3t}$
- 9. $F(t) = ae^{bt}$.
- 10. $F(t) = a\cos(\beta t + \gamma)$.
- 11. $F(t) = at^2 + 1$.

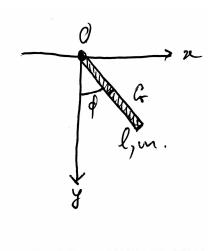


Figure 7: Illustration of a rotating rod around the origin, with center of gravity at G.

Rigid body motions

For this section, the main focus would be on rigid objects' rotational motions, kind of. One of the major preliminary knowledge that should be recalled is the inertia I of certain mass objects. Here, we recite them a bit. For

$$I = \sum_{i} m_{i} r_{i}^{2}, \quad I = \int r^{2} dm \tag{4.198}$$

we have the following amount:

$$I = \frac{ml^2}{12} \quad \text{(Long rod with midpoint rotating axis)} \tag{4.199}$$

$$I = \frac{mR^2}{2}(\text{Disk}) \tag{4.200}$$

$$I = mR^2 \quad \text{(Thin ring)} \tag{4.201}$$

$$I=rac{2}{5}mR^2$$
 (Solid sphere) (4.202)
$$I=rac{2}{3}mR^2 ext{(Surface sphere)} ext{(4.203)}$$

$$I = \frac{2}{3}mR^2(\text{Surface sphere}) \tag{4.203}$$

From this, we can then proceed to solve our particular problem of interest in this chapter: formulating the kinetic energy of such object. Let's have a look. Though first, let us know that we have the following formula for kinetic energy of rigid bodies:

$$T = \frac{1}{2}m\vec{v}^2 + \frac{1}{2}I\vec{\Omega}^2 \tag{4.204}$$

Here, $\vec{\Omega} = d\vec{\phi}/dt$ in a rotational manner.

Swinging rod

Alright, so it is formulated as below. Or rather, let's look at the diagram for such case: There, we have the coordinate at G as:

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$$\begin{pmatrix} x_G \\ y_G \end{pmatrix} = \begin{pmatrix} (l/2)\sin\phi \\ (l/2)\cos\phi \end{pmatrix} , \quad \begin{pmatrix} \dot{x}_G \\ \dot{y}_G \end{pmatrix} = \begin{pmatrix} (l/2)\dot{\phi}\cos\phi \\ (l/2)\dot{\phi}\sin\phi \end{pmatrix}$$
 (4.205)

The kinetic energy translational component is then:

$$T_{TT} = \frac{1}{2}m(\dot{x}_G^2 + \dot{y}_G^2)$$

$$= \frac{1}{2}m\left[\left(\frac{l}{2}\dot{\phi}\cos\phi\right)^2 + \left(-\frac{l}{2}\dot{\phi}\sin\phi\right)^2\right]$$

$$= \frac{m\dot{\phi}^2 l^2}{8}$$
(4.206)

The rotational kinetic energy is accordingly the following:

$$T_{Q} = \frac{1}{2}I\Omega^{2}$$

$$= \frac{1}{2}I\dot{\phi}^{2}$$

$$= \frac{1}{2}\frac{ml^{2}}{12}\dot{\phi}^{2}$$

$$= \frac{1}{24}ml^{2}\dot{\phi}^{2}$$
(4.207)

The kinetic energy in total is hence:

$$T = T_{TT} + T_Q = \frac{m\dot{\phi}^2 l^2}{8} + \frac{1}{24}ml^2\dot{\phi}^2 = \frac{1}{6}ml^2\dot{\phi}^2$$
 (4.208)

which is fairly nice, and you can simplify it pretty easily.

Rod attached of a thin disc

The next case we would be considering, is the case of the rod attached to a thin disc of no mass at the end. Here, we have two cases: either $m\approx 0$ or m is substantial energy to include its term into the equation. Nevertheless, we solve the first case, for m=0. Thence, the kinetic energy of the rod is zero, and we proceed with coordinate decomposition for the disc. Here, it is:

$$\begin{pmatrix} x_D \\ y_D \end{pmatrix} = \begin{pmatrix} (l+R)\sin\phi \\ (l+R)\cos\phi \end{pmatrix} , \quad \begin{pmatrix} \dot{x}_D \\ \dot{y}_D \end{pmatrix} = \begin{pmatrix} (l+R)\dot{\phi}\cos\phi \\ -(l+R)\dot{\phi}\sin\phi \end{pmatrix}$$
(4.209)

The translational kinetic energy is then:

$$T_{TT} = \frac{1}{2}M\bar{v}^{2}$$

$$= \frac{1}{2}M(\dot{x}^{2} + \dot{y}^{2})$$

$$= \frac{1}{2}M\left[\left((l+R)\dot{\phi}\cos\phi\right)^{2} + \left(-(l+R)\dot{\phi}\sin\phi\right)^{2}\right]$$

$$= M\frac{\left[\dot{\phi}(l+R)\right]^{2}}{2}$$
(4.210)

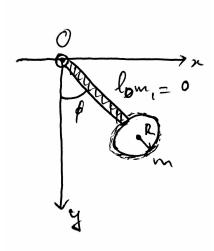


Figure 8: Illustration of a rotating rod around the origin, attached to a thin disc of radius R and of mass M. the rod has mass m and length l.

The rotational energy is:

$$T_Q = \frac{1}{2}I\Omega^2$$

$$= \frac{1}{2}\frac{MR^2}{2}\dot{\phi}^2$$

$$= \frac{1}{4}MR2\dot{\phi}^2$$
(4.211)

Hence, the kinetic energy is

$$T = T_{TT} + T_Q = M \frac{\left[\dot{\phi}(l+R)\right]^2}{2} + \frac{1}{4}MR2\dot{\phi}^2$$
 (4.212)

Now, if m of the rod is substantial, then we only have to add them in. In such case, we use the previous result already. Hence, we have:

$$\Sigma T = T_R + T_D = \frac{1}{6}ml^2\dot{\phi}^2 + M\frac{\left[\dot{\phi}(l+R)\right]^2}{2} + \frac{1}{4}MR2\dot{\phi}^2$$
 (4.213)

Somewhat a pendulum

Alright, let's take a look at this: Here, the rod mass is literally zero, so the entire system will again only have the quantification for the hanging dense sphere of mass m uniformly distributed. Hence, we have:

$$\begin{pmatrix} x_D \\ y_D \end{pmatrix} = \begin{pmatrix} (l+R)\sin\phi \\ (l+R)\cos\phi \end{pmatrix} , \quad \begin{pmatrix} \dot{x}_D \\ \dot{y}_D \end{pmatrix} = \begin{pmatrix} (l+R)\dot{\phi}\cos\phi \\ -(l+R)\dot{\phi}\sin\phi \end{pmatrix}$$
 (4.214)

Then,

$$T_G = \frac{1}{2}M\left[\dot{\phi}(l+R)\right]^2 \tag{4.215}$$

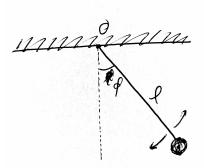


Figure 9: Illustration of a rotating rod around the origin, attached to a thin disc of radius R and of mass M. the rod has mass m and length l.

Now, for the translational kinetic energy, we gain:

$$\begin{split} T_Q &= \frac{1}{2} I \Omega^2 \\ &= \frac{1}{2} I \dot{\phi}^2 \\ &= \frac{1}{2} \frac{2}{5} M R^2 \dot{\phi}^2 \\ &= \frac{1}{5} m R^2 \dot{\phi}^2 \end{split} \tag{4.216}$$

The total kinetic energy is hence

$$T = T_{TT} + T_Q = \frac{1}{2}M\left[\dot{\phi}(l+R)\right]^2 + \frac{1}{5}mR^2\dot{\phi}^2 \tag{4.217}$$

If it is instead for (l-R), that is, the rotating 'pendulum' is with rod/line connected to the center of the sphere instead, then we have the following coordinates.

$$\begin{pmatrix} x_D \\ y_D \end{pmatrix} = \begin{pmatrix} (l-R)\sin\phi \\ (l-R)\cos\phi \end{pmatrix} , \quad \begin{pmatrix} \dot{x}_D \\ \dot{y}_D \end{pmatrix} = \begin{pmatrix} (l-R)\dot{\phi}\cos\phi \\ -(l-R)\dot{\phi}\sin\phi \end{pmatrix}$$
(4.218)

Hence, the kinetic energy is:

$$T_{\text{trans}} = \frac{1}{2} M \left[\dot{x}_D^2 + \dot{y}_D^2 \right] = \frac{1}{2} M \left((l - R)^2 \dot{\phi}^2 \right) = \frac{1}{2} M \left(l - R \right)^2 \dot{\phi}^2$$
 (4.219)

and,

$$T_{\text{rot}} = \frac{1}{2} I \dot{\phi}^2 = \frac{1}{2} \frac{2}{5} M R^2 \dot{\phi}^2 = \frac{1}{5} M R^2 \dot{\phi}^2$$
 (4.220)

The total kinetic energy is:

$$T = T_{\text{trans}} + T_{\text{rot}} = \frac{1}{2} M (l - R)^2 \dot{\phi}^2 + \frac{1}{5} M R^2 \dot{\phi}^2$$
 (4.221)

Grapple

The grapple situation is pretty crazy. For now though, we have the following situation to deal with: The linkage system forms a "V" shape, has two motions: B translational on Ox, and

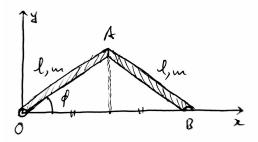


Figure 10: The isosceles triangle linkage system with length l, mass m on both side, and has two center of mass G_1 and G_2 on both rigid rods. In reduced notation, we use G, G'.

OA rotates around O. The coordinate components are then:

$$\begin{pmatrix} x_G \\ y_G \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\cos\phi \\ \frac{1}{2}\sin\phi \end{pmatrix} \quad , \quad \begin{pmatrix} \dot{x}_G \\ \dot{y}_g \end{pmatrix} = \begin{pmatrix} -\frac{1}{2}\dot{\phi}\sin\phi \\ \frac{1}{2}\dot{\phi}\cos\phi \end{pmatrix} \tag{4.222}$$

and

$$\begin{pmatrix} x_{G'} \\ y_{G'} \end{pmatrix} = \begin{pmatrix} \frac{3}{2}l\cos\phi \\ \frac{1}{2}\sin\phi \end{pmatrix} , \quad \begin{pmatrix} \dot{x}_{G'} \\ \dot{y}_{G'} \end{pmatrix} = \begin{pmatrix} -\frac{3}{2}l\dot{\phi}\sin\phi \\ \frac{1}{2}\dot{\phi}\cos\phi \end{pmatrix}$$
 (4.223)

Translational and rotational motions both are hence:

$$T = \frac{1}{2}m\left(\dot{x}_{G}^{2} + \dot{y}_{G}^{2}\right) + \frac{1}{2}I_{G}\dot{\phi}^{2} + \frac{1}{2}m\left(\dot{x}_{G'}^{2} + \dot{y}_{G'}^{2}\right) + \frac{1}{2}I_{G'}\dot{\phi}^{2}$$

$$= \frac{1}{2}m\left(\left(\frac{l}{2}\dot{\phi}\right)^{2}\right) + \frac{1}{2}\left(\frac{ml^{2}}{12}\right)\dot{\phi}^{2} + \frac{1}{2}m\left(\left(\frac{3l}{2}\dot{\phi}\right)^{2}\right) + \frac{1}{2}\left(\frac{ml^{2}}{12}\right)\dot{\phi}^{2}$$

$$= \frac{1}{2}m\frac{l^{2}}{4}\dot{\phi}^{2} + \frac{ml^{2}}{24}\dot{\phi}^{2} + \frac{1}{2}m\frac{9l^{2}}{4}\dot{\phi}^{2} + \frac{ml^{2}}{24}\dot{\phi}^{2}$$

$$= \left(\frac{1}{8} + \frac{1}{24} + \frac{9}{8} + \frac{1}{24}\right)ml^{2}\dot{\phi}^{2} = \frac{4}{3}ml^{2}\dot{\phi}^{2}.$$

$$(4.224)$$

Rolling wheel of thunder

A bit cringe, but here we go: Here, again we have the old $T_T + T_D$ of rotational and translational kinetic energy. However, the velocity in the translational case this time depends on the angular velocity $\dot{\phi}$, plus the distance from the center since it is indeed rolling around. Hence, of the law of Cosine, then:

$$d^{2} = a^{2} + R^{2} - 2aR\cos\phi \Rightarrow d = \sqrt{a^{2} + R^{2} - 2aR\cos\phi}$$
 (4.225)

So,

$$v = \dot{\phi}\sqrt{a^2 + R^2 - 2aR\cos\phi} \tag{4.226}$$

The kinetic energy in total is hence:

$$T = \frac{1}{2}m \left[\dot{\phi} \sqrt{a^2 + R^2 - 2aR\cos\phi} \right]^2 + \frac{I}{2} \dot{\phi}^2$$
 (4.227)

Notice that we do not have the explicit form of I. This is because there exists no such inertia calculation since the mass is not uniformly distributed, and can be distributed based on the condition only – as seen with the arbitrary distance a. However, this is usually enough.

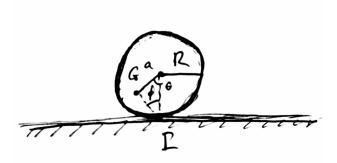


Figure 11: Illustration of a cylinder on the top cross-section of radius R rolling on the surface. The mass is not uniformly distributed, and hence is distributed such that there is an inertial axis that is of distance a from the center axis of the cylinder.

Hamiltonian and its equation

In this section, we tackle the other brother in the family, the Hamiltonian (mechanics). We can construct it from the Lagrangian, fortunately, so considering this it would be much easier for us to set up examples and derivations thereof for the set of Hamiltonian equations. For now, let's recall the Hamiltonian form as the following:

$$\mathcal{H}(q_i, p_i, t) = \sum_{i=1}^{s} p_i \dot{q}_i - \mathcal{L} = \sum_{i=1}^{s} p_i \dot{q}_i - \frac{1}{2} m \vec{v}^2 + U(q_i)$$
(4.228)

While Lagrangian is expressing a system via generalized coordinate and velocity, Hamiltonian expresses the system via its generalized coordinates and its generalized momenta instead, using what is called the Legendre transformation. The set of Hamilton equations is then:

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} \quad , \quad \dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}$$
 (4.229)

Hamiltonian from Lagrangian

Remember the momentum (momenta) from Lagrangian problem in the section on conservation law? We are going back, but this time, using the momentum to derive the results of a Hamiltonian form. Now, let's recall that we have the same Lagrangian:

$$\mathcal{L} = \frac{1}{2}m(\alpha^2 + \beta^2)(\dot{\alpha}^2 + \dot{\beta}^2) + \frac{1}{2}m\alpha^2\beta^2\dot{\gamma}^2$$
 (4.230)

To find the momenta of this Lagrangian, simply take the partial derivative w.r.t. to each individual generalized velocity:

$$p_{\alpha} = \frac{\partial \mathcal{L}}{\partial \dot{\alpha}} = m(\alpha^2 + \beta^2)\dot{\alpha}$$
$$p_{\beta} = \frac{\partial \mathcal{L}}{\partial \dot{\beta}} = m(\alpha^2 + \beta^2)\dot{\beta}$$
$$p_{\gamma} = \frac{\partial \mathcal{L}}{\partial \dot{\gamma}} = m\alpha^2\beta^2\dot{\gamma}$$

Here, we need the generalized velocity; but, since the momentum form already has the generalized velocity in it, we can then use algebraic manipulation to gain:

$$\dot{\alpha} = \frac{p_{\alpha}}{m(\alpha^2 + \beta^2)}, \quad \dot{\beta} = \frac{p_{\beta}}{m(\alpha^2 + \beta^2)}, \quad \dot{\gamma} = \frac{p_{\gamma}}{m\alpha^2\beta^2}$$
(4.231)

Hence, we can then gain the Hamiltonian as:

$$\mathcal{H} = \frac{p_{\alpha}}{m(\dot{\alpha}^2 + \beta^2)} m(\alpha^2 + \beta^2) \dot{\alpha} + \frac{p_{\beta}}{m(\dot{\alpha}^2 + \beta^2)} m(\alpha^2 + \beta^2) \dot{\beta} + \frac{p_{\gamma}}{m\alpha^2\beta^2} m\alpha^2\beta^2 \dot{\gamma} - \mathcal{L}$$
(4.232)

This can then be reduced to:

$$\mathcal{H} = p_{\alpha}\dot{\alpha} + p_{\beta}\dot{\beta} + p_{\gamma}\dot{\gamma} - \frac{1}{2}m(\alpha^2 + \beta^2)(\dot{\alpha}^2 + \dot{\beta}^2) - \frac{1}{2}m\alpha^2\beta^2\dot{\gamma}^2$$
(4.233)

Substitute the last generalized velocity in, we have:

$$\mathcal{H} = \frac{p_{\alpha}}{m(\alpha^{2} + \beta^{2})} m(\alpha^{2} + \beta^{2}) \frac{p_{\alpha}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\beta}}{m(\alpha^{2} + \beta^{2})} m(\alpha^{2} + \beta^{2}) \frac{p_{\beta}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}}{m\alpha^{2}\beta^{2}} m\alpha^{2}\beta^{2} \frac{p_{\gamma}}{m\alpha^{2}\beta^{2}} - \mathcal{L}$$

$$(4.234)$$

Which is:

$$\mathcal{H} = \frac{p_{\alpha}}{m(\alpha^{2} + \beta^{2})} m(\alpha^{2} + \beta^{2}) \frac{p_{\alpha}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\beta}}{m(\alpha^{2} + \beta^{2})} m(\alpha^{2} + \beta^{2}) \frac{p_{\beta}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}}{m(\alpha^{2} + \beta^{2})} m(\alpha^{2} + \beta^{2}) \frac{p_{\beta}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}^{2}}{m(\alpha^{2} + \beta^{2})} + \mathcal{L}$$

$$= \frac{p_{\alpha}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\beta}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}^{2}}{m(\alpha^{2} + \beta^{2})} - \mathcal{L}.$$

$$(4.235)$$

Hence, the Hamiltonian is:

$$\mathcal{H} = \frac{p_{\alpha}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\beta}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}^{2}}{m\alpha^{2}\beta^{2}} - \frac{1}{2}m(\alpha^{2} + \beta^{2})(\dot{\alpha}^{2} + \dot{\beta}^{2}) - \frac{1}{2}m\alpha^{2}\beta^{2}\dot{\gamma}^{2}$$
 (4.236)

Continue the simplification:

$$\mathcal{H} = \frac{p_{\alpha}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\beta}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}^{2}}{m\alpha^{2}\beta^{2}}$$

$$- \frac{1}{2}m(\alpha^{2} + \beta^{2})\left(\frac{p_{\alpha}^{2}}{m^{2}(\alpha^{2} + \beta^{2})^{2}} + \frac{p_{\beta}^{2}}{m^{2}(\alpha^{2} + \beta^{2})^{2}}\right)$$

$$- \frac{1}{2}m\alpha^{2}\beta^{2}\left(\frac{p_{\gamma}^{2}}{m^{2}\alpha^{4}\beta^{4}}\right)$$

$$= \frac{p_{\alpha}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\beta}^{2}}{m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}^{2}}{m\alpha^{2}\beta^{2}}$$

$$- \frac{p_{\alpha}^{2} + p_{\beta}^{2}}{2m(\alpha^{2} + \beta^{2})} - \frac{p_{\gamma}^{2}}{2m\alpha^{2}\beta^{2}}$$

$$= \frac{p_{\alpha}^{2} + p_{\beta}^{2}}{2m(\alpha^{2} + \beta^{2})} + \frac{p_{\gamma}^{2}}{2m\alpha^{2}\beta^{2}}.$$
(4.237)

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