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An Overview of Computational Mathematical Physics: A Deep Dive on Gauge Theories

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Claremont McKenna College

An Overview of Computational Mathematical Physics:
A Deep Dive on Gauge Theories

submitted to
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by
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for
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Abstract

Over the course of a college mathematics degree, students are inevitably exposed to elementary physics. The derivation of the equations of motion are the classic examples of applications of derivatives and integrals. These equations of motion are easy to understand, however they can be expressed in other ways that students aren't often exposed to. Using the Lagrangian and the Hamiltonian, we can capture the same governing dynamics of Newtonian mechanics with equations that emphasize physical quantities other than position, velocity, and acceleration like Newton's equations do. Building off of these alternate interpretations of mechanics and understanding gauge transformations, we begin to understand some of the mathematical physics relating to gauge theories. In general, gauge theories are field theories that can have gauge transformations applied to them in such a way that the meaningful physical quantities remain invariant. This paper covers the buildup to gauge theories, some of their applications, and some computational approaches to understanding them.

1 Introduction

This paper was written as a senior thesis in mathematics under the guidance of Sam Nelson, a Professor of Mathematics at Claremont McKenna College for the Spring semester of 2019. I want to give a big thank you to the CMC Mathematical Sciences Department, Keck Science Department, the College, and Professor Nelson for their support and guidance throughout my undergraduate experience.

My primary goal with this paper is to introduce complicated mathematical concepts and apply them to the simplest physical problems. This allows deeper insight into the way the math works since little energy has to be spent understanding the motion of springs or falling objects. Once the simple examples are explained, then the difficult concepts are alluded to but not discussed in detail. This maintains the focus of the paper on the math rather than the physics. I structured the paper so that each concept builds off of prior concepts in a logical progression. The major topics covered are gauges, gauge theories, Lagrangians, Hamiltonians, and Hamiltonian lattice gauge theory. However, in order to build up to those main topics, I include several subsections that develop the necessary tools to formally derive the main results.

2 An Introduction to Gauge Theories

This section will cover the foundations of gauge theories beginning with an overview of the Lagrangian and continuing with a discussion of the implications of invariant Lagrangians. Following that we will cover symmetry groups, Lie groups, restrictions we can place on the Lagrangian, and gauge groups.

In general, gauge theories are a derivation of physical field theories that involve symmetry groups. These symmetry groups are transformations which leave an object invariant once acted upon. In a geometric context, a symmetry group of a triangle might look like rotations, reflections, or translations of the triangle. The object was acted upon, but ultimately remained invariant because nothing structurally was changed. Symmetric in the context of gauge theory is less tangible; it means that once our physical field is acted on by a set of transformations, the Lagrangian is invariant and the physics of the field is unchanged. Lagrangian invariance tells us that the important physical characterizations that the Lagrangian captures remain unchanged. For example, acted upon by a symmetry group, a particle should maintain the same energy.

2.1 Overview of the Lagrangian

The Lagrangian is fundamental to our understanding of field theories like gauge theories and Hamiltonian Field Theory. The dynamics that govern interactions between objects, particles, and space are all captured in elegantly simple expressions involving the Lagrangian. As an example, we'll look at a basic Lagrangian that appears in elementary mechanics

$$\mathcal{L} \equiv T - V$$

where T is the total kinetic energy of the system and V is the total potential energy of the system such that

$$T = \sum_{i=1}^n m_i v_i^2 \quad V = \sum_{i=1}^n V_i$$

Expressing a physical system in this way removes the clutter and system of equations that describes the forces on each individual object and instead deals with cumulative energies. Another advantage of using the Lagrangian over the standard equations of motion is that the Lagrangian can be expressed using a generalized coordinate system. This becomes advantageous with chaotic systems like the double pendulum, where rather than laboriously calculating an x and y component, one can simply look at the angles θ_1 and θ_2 each pendulum makes with respect to some $\theta = 0$.

This gives us that the Lagrangian in a classical system for a rigid bodied mass is

$$\mathcal{L} \equiv T - V = \frac{1}{2}m\dot{x}^2 - mgx$$

where x is our generalized coordinate, \dot{x} is the velocity of the object, m is the mass of the object, and g is the gravitational constant for Earth. A physical example of where this might be useful is in dealing with a pulley system with several atwood machines where the equations of motion would need to be expressed for each segment of the pulley system as a separate force but in the case of the Lagrangian, all that is needed is the energy of the system and a general coordinate.

Theorem: Let \mathcal{L} denote the Lagrangian of a system such that $\mathcal{L} \equiv T - V = \frac{1}{2}m\dot{x}^2 - mgx$. Then Lagrangian mechanics is a valid formalism of Newtonian mechanics such that we can derive the same equations of motion.

Proof: Beginning with the Euler-Lagrange equation from the calculus of variations,

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

$$\begin{aligned}\frac{d}{dt}(m\dot{x}) - (-mg) &= 0 \\ -mg &= m\ddot{x} \\ F &= ma\end{aligned}$$

which is consistent with Newton's second law of motion. From $F = ma$, we can isolate the acceleration a and integrate twice to get the equations of motion. Thus Lagrangian mechanics is a valid formalism for classical mechanics for a rigid body.

2.2 Invariant Lagrangians

Invariant Lagrangians are of particular importance to us because gauge theories arise from certain conditions held on the Lagrangian. In Lagrangian mechanics, for example, the Lagrangian captures the scalar delta between the kinetic energy and the potential energy. This means that regardless of our coordinate system, that scalar quantity is unchanged and leads to the same equations of motion, thus coordinate transformations leave the Lagrangian invariant. In electromagnetism, the electric and magnetic potential are independent of coordinate systems just like gravitational potential energy, thus both are also invariant. This understanding of the importance of invariance brings us to looking at Lie groups and bundles, which is our final step before we can fully understand gauges and gauge transformations.

2.3 Lie Groups, Bundles, and Gauge Groups

Now that we understand Lagrangians, we need to build up to an understanding of gauge groups. We need to briefly cover Lie groups and bundles. In general, a Lie group is a smooth manifold that can be parameterized locally in such a way that the group operations (closure, associativity, existence of an identity element, and invertibility) are smooth locally. More formally, we get the following definition:

Def 1: (Hamilton 1.1.4) A **Lie Group** is a group that is simultaneously a manifold so that the map

$$\begin{aligned}G \times G &\longrightarrow G \\ (g, h) &\longmapsto g \cdot h^{-1}\end{aligned}$$

is smoothly differentiable $\in C^\infty$ such that the manifold has 'continuous symmetry'.

To visualize what it means to have continuous symmetry, imagine a circle and a square on a table. If you rotate the circle an arbitrarily small amount δ , then the

circle looks unchanged. In contrast, however, if you rotate a square by that same δ then you visually have a different looking object. However, if you rotate a square by $\delta = \frac{\pi}{2}$, then of course that rotation will be symmetric to the original square. That is where the difference in continuous symmetry comes in: symmetric objects have discrete actions that remain symmetric whereas continuously symmetric objects have symmetry that is continuous. In a 3-dimensional sense, consider a sphere and a football, the sphere has continuous symmetry in all directions of rotation for arbitrarily small δ . However, if you're looking head on at the football, it might initially appear to have continuous symmetry since its cross section is a circle so rotations along that cross section are continuous. However, any rotations that aren't directly along that axis show that the football does not have continuous symmetry since length-wise it does not have symmetry for arbitrarily small rotations δ .

Now we shift our focus toward bundles as the final component we need to define and understand to finally formally define gauges and gauge groups.

Def 2: (Hamilton 4.1.1) Consider a map $\pi : E \mapsto M$ where π is onto between E and M and where $E, M \in C^\infty$. Now let the point $x \in M$ be any arbitrary element of M , then the **fibre** of π over x is the subset

$$E_x = \pi^{-1}(x) = \pi^{-1}(\{x\}) \subset E$$

Def 3: (Hamilton 4.1.2) Consider manifolds E, F, M and $\pi : E \mapsto M$ where π is onto between E and M and where $E, M \in C^\infty$. Then $(E, \pi, M; F)$ is called a **fibre bundle** if the following condition holds: $\forall x \in M, \exists U \subset M$ where $U = N_\epsilon(x)$ such that π restricted to E_U can be trivialized, i.e. there exists a diffeomorphism $\phi \in C^\infty$ and $\phi^{-1} \in C^\infty$

$$\phi_U : E_U \mapsto U \times F$$

such that

$$\text{pr}_1 \circ \phi_U = \pi$$

The following are some examples of fibre bundles:

(1) Consider a cube. We can think of the base space as $\{(x, y) : 0 < x < l, 0 < y < l\}$, a square with sides l . Then the fibre is the interval $z = [0, l]$ and so we map the square to the fibre which projects each point of the square vertically for the interval $[0, l]$, yielding a cube of side length l . This is an example of a trivial bundle since the fibre is just an interval.

(2) Consider the same base space $\{(x, y) : 0 < x < l, 0 < y < l\}$. Now if the fibre takes points through $\{(x, y, z) : x = \cos(t), y = \sin(t), z = t\}$

then the fibre takes points through a helix, or ‘corkscrew’ in a 3rd dimension and we get a spiraling square (this looks like those stacks of Post-It notes that spiral upward). This is an example of a non-trivial bundle.

Now that we have a framework for Lie groups, fibres, bundles, and examples of each, we can start to understand gauges and gauge groups. Terence Tao colloquially describes gauges as the following:

Def 4: (Terence Tao) A **gauge** is nothing more than a ‘coordinate system’ that varies based on a particle’s location with respect to a base, parameterized space.

A gauge can be used to reduce the complexity of calculation (regulating redundant degrees of freedom in \mathcal{L}) by temporarily changing a coordinate system to be normalized. Consider a *coordinate-invariant* system where we can convert geometric quantities to a numeric quantity but all statements are invariant under changes in coordinates. This lets us take a quantity, say $|AB|$, that continually appears and let $|AB| = 1$ and reduce the complexity of the problem. However, statements like $|AB| = 1$ is not necessarily a true statement under a new coordinate system. Something like the Pythagorean Theorem $|AC|^2 = |AB|^2 + |BC|^2$ for a right triangle, however, is a true statement in any coordinate system, thus the Pythagorean Theorem is coordinate invariant. We can regulate our calculations by normalizing one quantity per degree of freedom in the symmetry group (Tao). A gauge is a way to use the invariance of objects under coordinate transformations to simplify calculations.

As another example of a gauge, consider a baseball thrown with sideways spin. Ignoring the complexities of fluid dynamics, at each point on the ball there is a positive or negative drag force vector from air resistance that runs in the direction of the spin. At every point on the baseball we can define a function $d(x, y, z)$ that gives the direction of the drag vector at that point. We could orient $d = 0$ to be either the true north of the ball or the direction of the spin or anything in between. This choice of gauge changes our direction function d , but is such that none of the physical quantities or information at any point on the ball is lost.

Now, we’ll formally define a gauge group to be the following

Def 5: (Hamilton 5.3.1) First suppose we have a map $\pi : P \rightarrow M$ be a principal G -bundle. A **gauge group**, denoted $\mathcal{G}(p)$, is a group formed by the composition of bundle automorphisms of P , a principal bundle (a bundle where the fibre is a group). This is equivalent to a diffeomorphism $f : P \rightarrow P$ which preserves the fibres of P and is

G -invariant where the following conditions hold.

1. $\pi \circ f = \pi$
2. $f(p \cdot g) = f(p) \cdot g \quad \forall p \in P \text{ and } g \in G$

Put more simply, gauge groups are Lie groups of a principal bundle's automorphisms.

To make the definitions more concrete, consider a coordinate system $\Phi : A \rightarrow G$ which takes a geometric object A and identifies it as an isomorphism of a standard object G . Now if we take any isomorphism of G which we call $\Psi : G \rightarrow G$. Then we can create a new coordinate system $\Psi \circ \Phi : A \rightarrow G$ by composing the isomorphism of G with the coordinate system. Every possible coordinate system Φ_i of A is formed by taking an isomorphism of G and composing it with Φ . This tells us that the space of coordinate systems of A is identifiable with the group of isomorphisms of G . This group of isomorphisms is the **gauge group** of the class of geometric objects (Tao). To make the idea more concrete, consider Φ that relates A the circle $|z| = n$, $n \in \mathbb{R}^+$, to G the unit circle $|z| = 1$. Then the gauge group would be the group of coordinate systems formed by relating circles of all radii to the unit circle.

2.4 Group Actions

In this section, we begin to look at the ways in which gauges appear in physics and how they are helpful. Lie groups and gauge groups have several ways in which they can act as transformation or symmetry groups on geometric objects (Hamilton p. 127). This is one of the areas in physics where gauges are most helpful since electromagnetism is gauge invariant. As physicists were trying to develop physics for particles and looking at the strong and weak interaction, gauge invariance and gauge groups were important since the ease of coordinate shifting lent itself well to developing more simple models. Physicists wanted to develop theories based on the action of gauge groups and symmetry groups of particles (Pickering p. 159, 164). An action can be thought of as a way of examining how a group's elements correspond to transformations of a space which preserves the structure of the space, so it has the same equivalence relations, measures, etc.

Def 6: (Hamilton 3.2.1) A **left-action** of a group G on a set M is a map

$$\Phi : G \times M \longrightarrow M$$

$$(g, p) \longmapsto \Phi(g, p) = g \cdot p = gp$$

which satisfies the following properties:

1. $(g \cdot h) \cdot p = g \cdot (h \cdot p)$ for all $p \in M$ and $g, h \in G$
2. $e \cdot p = p$ for all $p \in M$

Def 7: (Hamilton 3.2.2) A **right-action** of a group G on a set M is a map

$$\Phi : M \times G \longrightarrow M$$

$$(p, g) \longmapsto \Phi(p, g) = p \cdot g = pg$$

which satisfies the following properties:

1. $(p \cdot g) \cdot h = p \cdot (g \cdot h)$ for all $p \in M$ and $g, h \in G$
2. $p \cdot e = p$ for all $p \in M$

While we have defined separately left and right-actions, we can show that either can be converted to the other in the following theorem:

Theorem: Suppose, without loss of generality, we have a left action of a group G on M :

$$\Phi : G \times M \longrightarrow M$$

$$(g, p) \longmapsto \Phi(g, p) = g \cdot p = gp$$

Then the following defines a right action on M :

$$\Phi : M \times G \longrightarrow M$$

$$(p, g) \longmapsto \Phi(p, g) = p * g = g^{-1} \cdot p$$

Proof: Suppose we have defined $(p, g) \longmapsto \Phi(p, g) = p * g = g^{-1} \cdot p$. Then, from the notion that inversion changes the order of composition, we get

$$(g \cdot h) \cdot p = g \cdot (h \cdot p) = (p \cdot h^{-1}) \cdot g^{-1} = p \cdot (h \cdot g)^{-1} = (h \cdot g) \cdot p$$

which shows us that left-actions can be rewritten as right-actions and vice versa. This is similar to relating $\sin(x) = \cos(\frac{\pi}{2} - x)$. The theorem tells us that it isn't important which type of action we're given because we can transform it into another, just as it is not particularly important whether we are working with sin or cos in trigonometry because they are convertible.

Now that we've seen that left and right actions are in some sense the same, we can look at some of the more prevalent actions that arise in physics. Two particular types of action we'll look at are linear and Hopf actions.

Def 8: We have a **linear action** if the following holds true. Consider $\rho : G \rightarrow GL(V)$, a representation in a vector space V of a Lie group G .

$$\Phi : G \times V \longrightarrow V$$

$$(g, v) \longmapsto g \cdot v = \rho(g)v$$

The above is an example of a linear left-action, but as we saw from our previous theorem we can rework the example to be a linear right-action as well.

Turning our attention toward Hopf actions now, we quickly introduce the idea of a Hopf algebra and duality. In general, a Hopf algebra is simultaneously an algebra and coalgebra such that it is dual (for a sense of duality, Desargues' theorem in projective geometry is a good reference). This gives rise to nice commutative diagrams and symmetry.

Def 9: (Hamilton 3.3.1) Consider the groups \mathbb{R}^* , \mathbb{C}^* , and \mathbb{H}^* of non-zero real, complex, and quaternionic numbers. Let $\mathbb{K} = \mathbb{R}, \mathbb{C}, \mathbb{H}$ the following linear right actions, called **Hopf actions** by scalar multiplication:

$$\mathbb{K}^{n+1} \setminus \{0\} \times \mathbb{K}^* \longrightarrow \mathbb{K}^{n+1} \setminus \{0\}$$

Now when we look at elements of real, complex, and quaternionic numbers of unit norm on unit spheres we get the following Hopf actions

$$S^n \times S^0 \longrightarrow S^n$$

$$S^{2n+1} \times S^1 \longrightarrow S^{2n+1}$$

$$S^{4n+3} \times S^3 \longrightarrow S^{4n+3}$$

$$(x, \lambda) \longmapsto x\lambda$$

Before we can reach one of the most important results from group actions, we need to quickly define orbits and isotropy groups.

Def 10: Consider Φ , a left-action of a group G on a set M , then the **orbit** of G through a point $p \in M$ is given by

$$\mathcal{O}_p = G \cdot p = \{g \cdot p \mid g \in G\}$$

and the **isotropy group** of p is given by

$$G_p = \{g \in G \mid g \cdot p = p\}$$

Remark: When looking at a linear action, we can see that the orbit of the zero element of V (a vector space as opposed to M , a set) consists of only one point such that

$$G \cdot 0 = \{0\} \quad \text{since } \forall g \in G, g \cdot 0 = 0$$

which tells us that the isotropy group $G_0 = G$, that is the isotropy group of 0 is G itself. Thus when dealing with an element $v \in V$ such that $v \neq 0$ we get $G_v \subset G$. This means that we went from the entire group of G to a proper subset G_v . This is the very important idea of **symmetry breaking** in the standard model of quantum mechanics.

2.5 Restrictions on the Lagrangian

In theory, there exist an infinite number of Lagrangians that could model physical systems. However, we restrict them by particular principles to get a finite set. The Lagrangian and action of any individual field theory should be invariant under certain symmetry groups of gauge transformations.

Looking specifically at gauge groups, Hamilton demonstrates the importance of having Lagrangian invariance with respect to gauge symmetries. He showed that “a quantum field theory involving massless spin 1 bosons can be consistent, unitary, only if it is gauge invariant” (Hamilton p. 404). This leads to the restriction that Lagrangians be invariant under gauge symmetries.

The bracketed terms in the following Lagrangian are Lie brackets such that

$$[A, B] = AB - BA$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$

and now we define the YMDHY Lagrangian, the Lagrangian of the Standard Model.

Def 11: (Hamilton 7.1.4) We define the Lagrangian of the Standard Model as follows

$$\mathcal{L} = \mathcal{L}_D [\Psi, A] + \mathcal{L}_H [\Phi, A] + \mathcal{L}_Y [\Psi_L, \Phi, \Psi_R] + \mathcal{L}_{YM} [A]$$

which can be simplified to be

$$\mathcal{L} = \text{Re}(\bar{\Psi} D_A \Psi) + \langle d_A \Phi, d_A \Phi \rangle_E - V(\Phi) - 2g_Y \text{Re}(\bar{\Psi}_L \Phi \Psi_R) - \frac{1}{2} \langle F_M^A, F_M^A \rangle_{\text{Ad}(P)}$$

where \mathcal{L}_D is the Dirac Lagrangian, \mathcal{L}_H is the Higgs Lagrangian, \mathcal{L}_Y is the Yukawa Lagrangian, and \mathcal{L}_{YM} is the Yang-Mills Lagrangian. This causes the Lagrangian of the Standard Model to sometimes be referred to as the **Yang-Mills-Dirac-Higgs-Yukawa Lagrangian**.

The Standard Model Lagrangian attempts to describe the interactions between fundamental subatomic particles from the effects of the electromagnetic, gravitational, strong, and weak forces. The Standard Model is a gauge theory that expresses force interactions as changes in the Lagrangian. The fully factored out Lagrangian in **Def 11** contains kinetic, potential, and interaction terms between the different forces as they relate to gauge symmetries of the fundamental particles. Our build up of Lagrangians, Lie groups, bundles, gauges, and gauge groups culminates in this Standard Model Lagrangian which serves as a cornerstone of modern quantum mechanics. Again, this text is not meant to delve too deep into the physics of the Lagrangian, but rather to illuminate some of the mathematical structure governing it.

2.6 Gauge Theories

This section is the unification of our discussions on gauges, gauge groups, Lagrangians, and invariance. At a high level, a gauge theory is any field theory in which the Lagrangian is invariant under local gauge transformations. As we discussed above, the entire group of gauges which satisfies this condition form a gauge group (a special case of a Lie group). Physically this manifests itself as looking at all the ways in which a system can be redefined so that the underlying physics remains unchanged.

An example of a gauge theory which we are familiar with is electromagnetism. The basis of electromagnetism is formed by Maxwell's equations, given by the following system of equations

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)$$

Like most of the physics in this paper, the importance and derivation of these equations are outside our scope. We are interested in the relationship between the fields \mathbf{E} and \mathbf{B} and the scalar and vector potentials through which they can be re-expressed. The electric potential $V_{\mathbf{E}}$ and the magnetic potential \mathbf{A} are given by

$$V_{\mathbf{E}} = - \int_C \mathbf{E} \cdot d\mathbf{l}$$

$$\nabla \times \mathbf{A} = \mathbf{B}$$

These two equations show us that we could redefine Maxwell's equations in terms of $V_{\mathbf{E}}$ and \mathbf{A} if we wanted. However, there is some arbitrariness since we can slightly alter $V_{\mathbf{E}}$ and \mathbf{A}

with gauge transformations and leave \mathbf{E} and \mathbf{B} invariant. Another way to say this is that we have degrees of freedom in choosing how we define $V_{\mathbf{E}}$ and \mathbf{A} such that the resulting physics remains unchanged.

Consider the following example of a gauge transformation for electromagnetism. Let $\mathbf{A} \rightarrow \mathbf{A}'$ and $V_{\mathbf{E}} \rightarrow V'_{\mathbf{E}}$ then

$$\mathbf{A}'(\mathbf{x}', t) = \mathbf{A}(\mathbf{x}', t) - \nabla' f(\mathbf{x}', t) \quad (\text{Fitzpatrick 3.90})$$

$$V'_{\mathbf{E}}(\mathbf{x}', t) = V_{\mathbf{E}}(\mathbf{x}', t) + \frac{\partial f(\mathbf{x}', t)}{\partial t} \quad (\text{Fitzpatrick 3.91})$$

and this arbitrary function f leaves the magnetic and electric fields unchanged. Thus $\mathbf{A} \rightarrow \mathbf{A}'$ and $V_{\mathbf{E}} \rightarrow V'_{\mathbf{E}}$ is a gauge transformation and the electromagnetic field and its gauge group forms a gauge theory. This example gives us insight into how we can use gauge transformations with the degrees of freedom we have to redefine a system. As we'll see later with the Hamiltonian and lattice gauge theory, we can use these gauge transformations to obtain a partial differential equation to describe our system. This is advantageous because even if the exact solution is unknown, the PDE can give characteristics of the solution which can be a helpful analytical technique in understanding physical problems. Before we can take advantage of the Hamiltonian and lattice gauge theory, we need to understand Hamiltonians.

3 Hamiltonian Field Theory

Hamiltonian mechanics is a different formalism from Newtonian and Lagrangian mechanics. It predicts the same outcomes, but using a different mathematical structure. Hamiltonian mechanics represents a classical system with canonical coordinates $\mathbf{r} = (\mathbf{q}, \mathbf{p})$. We have that $\mathbf{q} = (q_1, q_2, \dots, q_n)$ is the generalized position and $\mathbf{p} = (p_1, p_2, \dots, p_n)$ is the generalized momentum (Prokhorov p. 1). A distinction between Hamiltonian mechanics and classical mechanics is that \mathbf{q} need not be rectangular coordinates. For example, a generalized coordinate might be an angle similar to polar coordinates or it could be a magnitude of distance from a reference point, etc. Additionally, these canonical coordinates gives an advantage over Lagrangian mechanics since with the Hamiltonian there is a canonical transformation that allows one to change the coordinates quickly and easily so that the system is simplified; we'll see how this is done later.

Hamiltonian field theory is the field theory pertaining to Hamiltonian mechanics. Hamiltonian mechanics differs from classical mechanics in that the Hamiltonian captures how the system changes over time and then that Hamiltonian is used in Hamilton's equations of motion. In classical mechanics, the equations of motion each directly and separately capture how the particular aspect of the system changes over time, i.e. acceleration over time vs. velocity over time vs. position over time.

3.1 Derivation of Hamilton's Equations

In this first section we want to show how one can derive consistent, but new equations of motion for a rigid body using the Hamiltonian. In general, Hamiltonian Mechanics are based off Hamilton's principle which states that

Def 12: (Prokhorov 1.1) **Hamilton's Principle** states that the equation of motion $q(t)$ with fixed end points $q(t_0)$ and $q(t_1)$ is an extremum of the action functional given by

$$S[q; t_0, t_1] = \int_{t_0}^{t_1} \mathcal{L}(\dot{q}, q, t) dt$$

where \mathcal{L} is the lagrangian of the system

From Hamilton's Principle, we get that the Euler Lagrange equation of motion for dynamical systems is given by

$$\frac{d}{dt} \frac{\partial}{\partial \dot{q}^i} \mathcal{L}(\dot{q}, q, t) = \frac{\partial}{\partial q^i} \mathcal{L}(\dot{q}, q, t) \quad (\text{Prokhorov 1.5})$$

This equation is derived from the fact that dynamical systems are described by Hamilton's Principle. We can describe a new variable

$$p^i = \frac{\partial}{\partial \dot{q}^i} \mathcal{L}(\dot{q}, q, t)$$

where p^i is the canonical momentum of q^i which gives us the canonical coordinates $\mathbf{r} = (\mathbf{q}, \mathbf{p})$ we introduced at the beginning of this section. Now using the Euler Lagrange equation along with p^i we get

$$\dot{p}^i = \frac{\partial}{\partial q^i} \mathcal{L}(\dot{q}, q, t)$$

Now in order to finish deriving Hamilton's equations, we need to define the following

Def 13: (Prokhorov p. 7) Given an equation

$$\mathbf{y} = \frac{\partial f}{\partial \mathbf{x}}$$

we can let $\mathbf{x} = \mathbf{x}(\mathbf{y})$ and get the following equation:

$$g(\mathbf{y}) = \mathbf{y} \cdot \mathbf{x}(\mathbf{y}) - f(\mathbf{x}(\mathbf{y}))$$

which is defined as the **Legendre transform** of f

Now we can define the Hamiltonian of a system and finish deriving Hamilton's equations

Def 14: (Prokhorov 1.23) The **Hamiltonian** of a system is the Legendre transform of $\mathcal{L}(\dot{q}, q, t)$ w.r.t. the variable \dot{q} and is given by

$$H(p, q, t) = p^i \dot{q}^i - \mathcal{L}(\dot{q}, q, t)$$

Now looking at the action functional of the Hamiltonian, we get

$$S_H = \int_{t_0}^{t_1} (p^i \dot{q}^i - H) dt$$

which is just a rewriting of the action functional from **Def 12** above using the relation in **Def 14**. Now to get Hamilton's equations of motion, we differentiate S_H w.r.t. the two independent variables p^i, q^i which gives

$$\frac{\delta S_H}{\delta p^i} = \dot{q}^i - \frac{\partial H}{\partial p^i}, \quad \frac{\delta S_H}{\delta q^i} = -\dot{p}^i - \frac{\partial H}{\partial q^i}$$

and once we set $\delta S_H = 0$ then we get

Def 15: (Prokhorov 1.25) **Hamilton's Equations of Motion** are given by

$$\dot{q}^i = \frac{\partial H}{\partial p^i}, \quad \dot{p}^i = -\frac{\partial H}{\partial q^i}, \quad \frac{\partial H}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}$$

Since p^i is the momentum of our particle in the i^{th} frame of reference, we can rewrite the Hamiltonian as the total energy in the system which gives

$$H = T + V \quad T = \frac{p^2}{2m} \quad V = V(q, t)$$

which gives us that $T = \frac{1}{2}m\dot{q}^2$, the kinetic energy, and V is the potential energy of the particle mass. If we want to extend this formulation to an arbitrary N number of particles, we simply get

$$H = \sum_{n=1}^N T_n + V$$

where T_n is the kinetic energy of the n^{th} particle and V is the potential energy function where $V = V(q_1, q_2, \dots, q_N, t)$.

Exercise: Derive Hamilton's equations for an oscillating mass

Solution: From elementary physics, we know that $T = \frac{1}{2}m\dot{q}^2$ and that $V = \frac{1}{2}kq^2$ where $k \in \mathbb{R}^+$. Now if we look at H we get that

$$H = \frac{1}{2}m\dot{q}^2 + \frac{1}{2}kq^2$$

Now if we take the derivative of T with respect to \dot{q} , we get

$$\frac{\partial T}{\partial \dot{q}} = \frac{\partial}{\partial \dot{q}} \left(\frac{1}{2}m\dot{q}^2 \right) = m\dot{q} = p$$

since p is the momentum of the particle and $m\dot{q}$ represents the momentum of an object. With some algebra, this coincides with above where we stated that $T = \frac{p^2}{2m}$. Substituting this into $H = T + V$ we get

$$H = \frac{p^2}{2m} + \frac{kq^2}{2}$$

And so once we apply Hamilton's equations to our oscillating system, we get

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m} + 0 = \frac{p}{m} \\ \dot{p} &= -\frac{\partial H}{\partial q} = -(0 + kq) = -kq \end{aligned}$$

And we can see that \dot{p} , which is the Newtonian force, agrees with the force for an oscillator from classical mechanics so our Hamiltonian derivation agrees with classical mechanics.

3.2 Canonical Transformations

As mentioned above, Hamiltonian mechanics is convenient because there is a formal way to redefine a coordinate system to simplify the complexity of a given system through canonical transformations.

Def 16: A **canonical transformation** is a change of canonical coordinates $(\mathbf{q}, \mathbf{p}, t) \rightarrow (\mathbf{Q}, \mathbf{P}, t)$ which preserves the form of Hamilton's equations, although not necessarily the Hamiltonian itself.

As we saw earlier for Hamilton's equations, we get that

$$\dot{\mathbf{q}}^i = \frac{\partial H}{\partial \mathbf{p}^i}, \quad \dot{\mathbf{p}}^i = -\frac{\partial H}{\partial \mathbf{q}^i}$$

and if we redefine new variables, \mathbf{Q} and \mathbf{P} , then we get for our new canonical equations

$$\dot{\mathbf{P}}^i = \frac{\partial K}{\partial \mathbf{P}^i}, \quad \dot{\mathbf{Q}}^i = -\frac{\partial K}{\partial \mathbf{Q}^i}$$

where K is a new Hamiltonian, since in our definition we noted that H is not necessarily invariant. This lets us redefine our coordinates in such a way that we preserve the form of Hamilton's equations, but with an alternate Hamiltonian.

3.3 Hamilton-Jacobi Equation

The Hamilton-Jacobi equation is notable since it is a way to use mechanics to describe the motion of a particle as a wave. It can also be used to identify conserved quantities in classical systems. The equation is linked to classical mechanics through the function S , defined below, which also happens to be the action of the particle. The Hamilton-Jacobi is a partial differential equation, which has the advantage of identifying certain attributes and characteristics of a system even when the explicit problem cannot be solved for completely (Chang).

Theorem: The **Hamilton-Jacobi equation** is given by

$$\partial_t u(\mathbf{q}, t) + H(\nabla_{\mathbf{q}} u(\mathbf{q}, t), \mathbf{q}) = 0$$

where u is a generating function giving time-dependent canonical transformations.

Proof(Based on Chang): Suppose we want to find a time-dependent canonical transformation where K , the transformed Hamiltonian is 0. Before we can derive such a K it will be helpful to have a relationship between the new and old Hamiltonians. Suppose we have a canonical transformation

$$(\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{Q}, \mathbf{P})$$

then there is a function S such that

$$S : \mathbb{R}_{\mathbf{q}}^n \times \mathbb{R}_{\mathbf{p}}^n \rightarrow \mathbb{R} \mid \mathbf{p} d\mathbf{q} - \mathbf{P} d\mathbf{Q} = dS$$

We know such a function exists because

$$d(\mathbf{p} d\mathbf{q} - \mathbf{P} d\mathbf{Q}) = d\mathbf{p} \wedge d\mathbf{q} - d\mathbf{P} \wedge d\mathbf{Q} = 0 \quad (\text{Chang 2.2})$$

where \wedge represents the wedge product. Since the differential is 0 then there exists an S . Now suppose that we want a time-dependent canonical transformation

$$(\mathbf{q}, \mathbf{p}, t) \rightarrow (\mathbf{Q}(\mathbf{q}, \mathbf{p}, t), \mathbf{P}(\mathbf{q}, \mathbf{p}, t), t)$$

then we can relate the new and old Hamiltonians with the following equation

$$K(\mathbf{Q}, \mathbf{P}, t) = H + \mathbf{P} \cdot \partial_t \mathbf{Q} + \partial_t S$$

Now suppose that

$$S = u(\mathbf{q}, \mathbf{P}(\mathbf{q}, \mathbf{p}, t), t) - \mathbf{Q}(\mathbf{q}, \mathbf{p}, t) \cdot \mathbf{P}(\mathbf{q}, \mathbf{p}, t)$$

where u is a generating function that gives time-dependent canonical transformations. Then the partial derivative of S with respect to time gives

$$\frac{\partial}{\partial t} S = \nabla_{t u} \cdot \partial_t \mathbf{P} + \partial_t u - \mathbf{Q} \cdot \partial_t \mathbf{P} - \mathbf{P} \cdot \partial_t \mathbf{Q}$$

$$\frac{\partial}{\partial t} S = \mathbf{Q} \cdot \partial_t \mathbf{P} + \partial_t u - \mathbf{Q} \cdot \partial_t \mathbf{P} - \mathbf{P} \cdot \partial_t \mathbf{Q}$$

$$\frac{\partial}{\partial t} S = \partial_t u - \mathbf{P} \cdot \partial_t \mathbf{Q}$$

And when we substitute this result into $K(\mathbf{Q}, \mathbf{P}, t) = H + \mathbf{P} \cdot \partial_t \mathbf{Q} + \partial_t S$ then we get that

$$K = H + \partial_t u$$

letting $K = 0$ and recognizing that the above equation has no dependence on \mathbf{P} , we get

$$\partial_t u(\mathbf{q}, t) + H(\nabla_{\mathbf{q}} u(\mathbf{q}, t), \mathbf{q}) = 0$$

and thus concludes the proof.

Remark: The Hamilton-Jacobi equation can be rewritten using the action functional as $\partial_t S = -H$

Exercise: Use the Hamilton-Jacobi equation to derive the equations of motion for a falling object

Solution: The Hamiltonian for a falling object is

$$H = \frac{1}{2m} p^2 + mgq$$

corresponding to the kinetic energy plus the gravitational potential energy. Next, we notice that H is not explicitly dependent on time since g , the force, is not time dependent. Relating H to a new Hamiltonian K by a generating function S as we did in the Hamilton-Jacobi equation derivation above, we get $\partial_t S + H = K$. Letting $K = 0$ so energy is conserved, we get

$$\frac{1}{2m} p^2 + mgq + \partial_t S = 0$$

Now if we have $p = \partial_q S$, i.e. the momentum equal to the partial derivative with respect to q of the generating function we get

$$\frac{1}{2m}(\partial_q S)^2 + mgq + \partial_t S = 0$$

Fortunately, this PDE is solvable and will generally have a solution of the form

$$S(c, q, t) = W(c, q) - ct$$

where W is an arbitrary function and c an arbitrary constant. This lets us rework the above equation to be

$$\frac{1}{2m}(\partial_q W)^2 + mgq - c = 0$$

Now we can solve the above differential equation for W to get

$$W = \int \sqrt{2m(c - mgq)} dq$$

So now we have an expression for S using our expression for W above

$$S(c, q, t) = \int \sqrt{2m(c - mgq)} dq - ct$$

where we have a new input c . This action S will make the Hamiltonian zero through a canonical transformation so if we look at $\partial_c S$ then we know it will be some constant γ .

$$\gamma = \partial_c S = \int \frac{\sqrt{m}}{\sqrt{2(c - mgq)}} dq - t \rightarrow \gamma = \sqrt{\frac{2(c - mgq)}{mg^2}} - t$$

and rearranging in terms of q we get the following

$$q = \frac{c}{mg} - \frac{(\gamma + t)^2 g}{2}$$

The above equation has some arbitrariness to it, so if we have initial conditions that $q(t = 0) = q_o$ so that our object starts falling from a height of q_o and if we let $p(t = 0) = 0$ so that our object has zero initial velocity. Then we have

$$p(t = 0) = 0 = \partial_q S = \sqrt{2m(c - mgq_o)}$$

So we get that at time $t = 0$, $c = mgq_o$. Replacing this and $\gamma = 0$ so that both our initial conditions are satisfied then we get

$$q = q_o - \frac{gt^2}{2}$$

which is also the classical solution for a falling object.

The above exercise shows both the usefulness of the Hamiltonian and also shows how the Hamilton Jacobi equation can be used to solve physical problems with rigid bodies. Next we'll quickly turn our focus to the Hamiltonian in quantum mechanics and use the wavelike properties that the Hamiltonian lends itself to.

3.4 The Hamiltonian in Quantum Mechanics

The point of this section is not to provide a thorough explanation of quantum mechanics but to introduce how the Hamiltonian can be useful in other areas of physics beyond mechanics. As we saw in the derivations and in the exercise above, the Hamiltonian leads to classically consistent results. However, the Hamiltonian also has useful applications to quantum mechanics because of its relationship with momentum. While the general derivation of the Hamiltonian is the same as our classical derivation, one key difference is that

$$\hat{p} = -i\hbar\nabla$$

which redefines momentum with a quantum mechanical definition. Using this new \hat{p} gives that the Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(q, t)$$

This formulation of the Hamiltonian is important because it allows it to be applied to systems described by the wave equation. Another way that Hamiltonian mechanics lends itself nicely to quantum mechanics is that the formulation deals with momentum more often than velocity, which is helpful for particle motion and the standard model. An example to demonstrate the usefulness of momenta versus velocities is the Heisenberg Uncertainty Principle which states that

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

the derivation or interpretation of the Principle is outside the scope of this paper but it is a cornerstone of quantum mechanics and demonstrates the importance of understanding momenta rather than velocity.

We saw above that

$$H = \sum_{n=1}^N T_n + V$$

where T_n is the kinetic energy of a particle and V is the potential energy of the system. If we take the *momentum* derivative of H , we get

$$\begin{aligned}\frac{\partial H}{\partial p} &= \frac{\partial}{\partial p} \left(\sum_{n=1}^N T_n + V \right) \\ \frac{\partial H}{\partial p} &= \frac{\partial}{\partial p} \left(\sum_{n=1}^N \frac{1}{2} m_n \dot{q}_n^2 + V \right) \\ \frac{\partial H}{\partial p} &= \frac{\partial}{\partial p} \left(\sum_{n=1}^N \frac{1}{2m_n} p_n^2 + V \right) \\ \frac{\partial H}{\partial p} &= \sum_{n=1}^N \frac{1}{m_n} p_n = \sum_{n=1}^N \frac{1}{m_n} m_n \dot{q}_n = \sum_{n=1}^N \dot{q}_n\end{aligned}$$

and this gives us an elegant relationship between the Hamiltonian and velocities, using the momentum. Moreover, if the derivative of the Hamiltonian with respect to momentum is derived with respect to time, we get acceleration. That is,

$$\frac{d}{dt} \frac{\partial H}{\partial p} = \frac{d}{dt} \sum_{n=1}^N \dot{q}_n = \sum_{n=1}^N \ddot{q}_n$$

These sections on Hamiltonian mechanics demonstrate some of its advantages over Lagrangian and classical mechanics. The Hamiltonian equations give us the equations of motion in terms of the derivatives with respect to momentum which is advantageous for quantum mechanics because as we saw with Heisenberg's Uncertainty Principle, the momentum of a particle is of particular importance for the standard model. Additionally, Hamiltonian mechanics is constructed at the particle-level and summed over all the particles in the phase space, whereas Newton's equations can only deal with a single body at a time. This is cumbersome for calculations over an entire system. Additionally, Hamiltonian mechanics lends itself to canonical coordinate changes which simplifies systems and calculations, which is a big advantage for modeling large groups of particle interactions. These advantages make the Hamiltonian useful for classical mechanics, quantum mechanics, thermodynamics, and other fields of physics.

4 Hamiltonian Lattice Gauge Theory

We've so far seen a lot of theoretical concepts and derivations. This final section shows the intersection between gauges and the Hamiltonian. Hamiltonian lattice gauge theory provides

a calculational approach to gauge theory using the Hamiltonian. As a brief overview, Hamiltonian lattice gauge theory discretizes space but not time. This then allows the Hamiltonian to be expressed on a multi-dimensional lattice.

4.1 Fermionic Fields on a Lattice

Consider a cubic lattice. Any arbitrary point on the lattice can be represented by $\vec{\mathbf{r}} = (\gamma_x, \gamma_y, \gamma_z)$. At each lattice site, let $\psi(\gamma)$ denote a two-component spinor.

Def 17: A **spinor** is a two component complex vector that describes fermions and is characterized by the way it behaves under rotations.

Then we can construct a Hamiltonian such that

$$H = a^{-1} \sum_{\gamma, n} \psi^\dagger(\gamma) \frac{\vec{\sigma} \cdot \vec{\mathbf{n}}}{i} \psi(\gamma + n) + m_o \sum_{\gamma} (-1)^\gamma \psi^\dagger(\gamma) \psi(\gamma) \quad (\text{Kogut 2.1})$$

where a represents the lattice spacing (the distance between each lattice site), \dagger represents the adjoint, γ represents an arbitrary radius, ψ represents a two-component spinor, $\vec{\sigma}$ is a Pauli vector, m_o is the rest mass, and $\vec{\mathbf{n}}$ is the outward unit norm.

Now consider a fermionic field, a quantum field whose quanta are fermions. The scope of fermionic fields is beyond this paper, but the general idea is that fermions (particles that have half-integer spin) follow Fermi-Dirac statistics, which explains a distribution of many identical particles over energy states that follow the Pauli exclusion principle. If we look at certain transformations of the spinors of the lattice, we get the following global and local gauge transformation definitions.

Def 18: (Kogut 2.6) Under a global gauge transformation, the transformed fermionic field is given by

$$\widehat{\psi}(\gamma) = e^{i\vec{\tau} \cdot \vec{\omega}/2} \psi(\gamma) \equiv V \psi(\gamma)$$

Under a global gauge transformation, we can see that the Hamiltonian is invariant since we've only multiplied $\psi(\gamma)$ by a constant $V \equiv e^{i\vec{\tau} \cdot \vec{\omega}/2}$ which doesn't change the interpretation of the Hamiltonian system. This is one of the advantages of using the Hamiltonian: we can change the coordinate system with which our lattice is defined by a global gauge transformation to make the system more simple. We have to be careful, however, because the Hamiltonian is *not* invariant under local gauge transformations which we define as

Def 19: (Kogut 3.1) Transforming the fermionic field by a local gauge transformation gives

$$\widehat{\psi}(\gamma) = e^{i\vec{\tau} \cdot \vec{\omega}(\gamma)/2} \psi(\gamma) \equiv V(\gamma) \psi(\gamma)$$

Under these transformations, we can see that V is now a function of γ which means that the Hamiltonian is no longer affected by a constant amount but rather depends on the specific lattice site under consideration. Intuitively this makes sense since a global transformation of the entire lattice shouldn't depend on any specific lattice site and a local transformation of an individual site *should* depend on a particular site.

In an effort to account for the Hamiltonian's local invariance, a gauge field $\vec{\mathbf{B}}(\gamma, n)$ is introduced, where (γ, n) is an individual link between lattice sites γ and n . We also introduce an operator U which preserves the inner product between two sites such that

$$U(\gamma, n) = e^{i\frac{1}{2}\vec{\sigma}\cdot\vec{\mathbf{B}}(\gamma, n)} \quad (\text{Kogut 3.2})$$

Here the gauge field is associated with the links between sites as opposed to the sites themselves. In that sense, the gauge field transfers information between points, like how an electric field transports charge. In this case, the gauge field transports color between points.

Def 20: In particle physics, **color charge** is a property of elementary particles that relates to the strong interactions in the theory of quantum chromodynamics. In chromodynamics one can draw color field lines much like how electric or magnetic fields can be drawn and this is the information the gauge field is transporting.

The equation above for $U(\gamma, n)$ is convenient because we can look at elements of the Hamiltonian and see that they are now invariant. Kogut gives the example of the operator

$$\psi^\dagger(\gamma)\psi(\gamma + n)$$

which was previously transformed under gauge transformations to

$$\psi^\dagger(\gamma)V^{-1}(\gamma)V(\gamma + n)\psi(\gamma + n)$$

and is clearly not gauge invariant because of the terms $V^{-1}(\gamma)V(\gamma + n)$. However, when we transform the operator to become

$$\psi^\dagger(\gamma)U(\gamma, n)\psi(\gamma + n)$$

then it *is* gauge invariant. Now we introduce this change to the Hamiltonian of the system to make the entire Hamiltonian locally and globally gauge invariant:

$$H = a^{-1} \sum_{\gamma, n} \psi^\dagger(\gamma) \frac{\vec{\sigma} \cdot \vec{\mathbf{n}}}{i} U(\gamma, n) \psi(\gamma + n) + m_o \sum_{\gamma} (-1)^\gamma \psi^\dagger(\gamma) \psi(\gamma) \quad (\text{Kogut 3.5})$$

And thus we have used an operator transform to make our Hamiltonian locally and globally gauge invariant. This section shows that regardless of whether the Hamiltonian is gauge invariant, there is a method in place when using lattices of particles to redefine the Hamiltonian to be gauge invariant.

4.2 Gauge-Field Hamiltonian

In order to ensure local gauge invariance, the Hamiltonian must be composed of gauge-invariant operators. One such operator we looked at briefly before is U . There are other methods which Kogut covers that can induce gauge invariance in a Hamiltonian. However, the methods are involved and require complex physical explanation so this paper doesn't go into them. Combining all of these disparate components into a unified equation, we get the following Hamiltonian.

Def 21: (Kogut 6.6) The **Gauge Field Hamiltonian** is defined to be

$$H = \frac{a}{2g^2} \sum_{r,m} \dot{B}^2(\gamma, m) + \frac{4}{ag^2} \sum \text{tr}U(\gamma, n)U(\gamma + n, m)U(\gamma + n + m, -n)$$

$$U(\gamma + m, -m) + a^{-1} \sum \psi^\dagger(\gamma) \frac{\vec{\sigma} \cdot \vec{n}}{i} U(\gamma, n) \psi(\gamma + n) + m_o \sum (-1)^\gamma \psi^\dagger(\gamma) \psi(\gamma)$$

such that H is invariant under both local and global gauge transformations, completing our formulation of a gauge theory.

This section on the Hamiltonian formulation of lattice gauge theories covers very complicated physical topics. The gauge field Hamiltonian covers enough physics for an entire paper by itself; the physics is not the point of this section of the paper. Rather, we are trying to illuminate the uses of some of the mathematical concepts that we have covered earlier in the paper. This section on lattice gauge theories uses many of the ideas we covered earlier in the paper from invariance to Hamiltonians to gauges into a singular application.

Conclusion

As I mentioned at the beginning of the paper, this is not meant to be an exhaustive text on the topics. My primary intention was to define and understand the mathematical concepts, briefly explain their significance, and then apply them to very simple physical situations. When I introduced more complicated topics like the Standard Model Lagrangian or the Gauge Field Hamiltonian, they were mostly to illustrate that the math *could* be applied to those complicated situations. The main topics of the paper are Lagrangians, gauges, gauge groups and theories, and Hamiltonians. Each of these required several subsections to build up to their formal definitions. I accompanied each of these topics with physical applications and included calculational examples where they made sense. The final section of the paper on Hamiltonian lattice gauge theory is the culmination of all of the seemingly disparate topics we covered. It showed us how gauges and invariance can be linked to the Hamiltonian and how that can provide calculational applications to gauge theories in quantum mechanics.

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