# PHYS624 Notes

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# 1 Motivation

Why do we need QFT? Consider a problem we already know, the Hydrogen atom. Consider an electron in the $2s$ state. If we wait long enough, it will decay to the $1s$ state. How long does it take for the electron to decay to decay from $2s \to 1s$? In QM, we spent time computing the energy splitting between the two states, which sets the frequency of the Lyman line. We never posed the question of how long it takes to transition between the two states. The reason for this is that in non-relativistic QM, the transition time is infinite, these are stationary states, they never decay. Since both mass and energy are conserved separately, the decay process

$$2s \to 1s + \text{photons}$$

can never occur, since particle number is conserved in non-relativistic QM. Usually in non-relativistic QM, we begin with a particle and we maintain that particle, the norm of the particle's wavefunction is conserved in time. In this case, we have photons that come into being, and we need some formalism that allows us to describe processes like this. Let us write down the Schrodinger equation for the Hydrogen atom:

$$\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{r},t) - \frac{e^2}{r}\psi(\boldsymbol{r},t) = i\hbar\frac{\partial\psi}{\partial t}$$

We have a wavefunction that describes the electron, and the $\frac{e^2}{r}$ term comes from the electromagnetic field, and we are treating this field completely classically, we are using the classical Coulomb potential. The photons are quantum objects, and they are excitations in the EM field, which means we need to treat them quantum mechanically. Just like we quantized the motion of the electron into $\psi(\boldsymbol{r},t)$, we need to quantize the EM field in order to obtain a quantum mechanical formalism for the decay process.

QFT has many subtleties, but there is a central idea that we want to highlight. In QM, we discuss wave-particle duality: if we quantize the motion of particles, we observe wave behavior. What we will see in this course is that if we quantize the motion of waves, we get particles, the duality holds bidirectionally. Most of this course will be exploring the quantization of waves and how they generate particles.

What does this other direction of the duality mean? For every particle we think of in nature, we can start with a field description, and each particle will be an excitation of the field, i.e. an electron is an excitation of the electron field.

There are three ingredients that go into QFT:

1. Non-relativistic quantum mechanics
2. Special Relativity
3. Classical field theory

With these three things, we can produce relativistic quantum field theory. In fact, we can pick any of two of these, and we have a consistent subject. For example, if we put non-relativistic QM and special relativity together, we get relativistic QM. If we put classical field theory and special relativity together, we get relativistic classical field theory (such as E&M). Finally, if we put non-relativistic QM together with classical field theory, we will get non-relativistic QFT.

In this course, we will choose to discuss classical field theory and special relativity, to obtain relativistic classical field theory. We will then consider relativistic QM, then non-relativistic QFT, and then finally we will put them all together to look at relativistic QFT.

# 2 Classical Field Theory

*This discussion is taken from the last chapter of Goldstein.*

## 2.1 Discrete Systems

We can think of classical field theory as the mechanics of continuous media. The way we approach a continuous system is to take it as the limit of a discrete system with many degrees of freedom, we take the continuum limit to recover the continuous system.

Consider an infinitely long elastic rod that undergoes longitudinal vibrations, that is, compression waves. We will approximate this as an infinite chain of point masses spaced a distance $a$ apart, connected by massless springs with spring constant $k$:



Suppose we have a vibration along this chain, we displace the masses from their equilibrium positions. We label the displacements by $\eta$, and we index each mass, that is, the displacement of the $i$th mass is $\eta_i$. At equilibrium, $\eta_i = 0$ for all $i$.

We can write down the kinetic energy in the chain:

$$T = \frac{1}{2}m\sum_i \dot{\eta}_i^2$$

And the potential energy:

$$V = \frac{1}{2}k\sum_i \left(\eta_{i+1} - \eta_i\right)^2$$

And then write down the Lagrangian:

$$\begin{aligned} L &= T - V \\ &= \frac{1}{2}\sum_i \left[m\dot{\eta}_i^2 - k\left(\eta_{i+1} - \eta_i\right)^2\right] \end{aligned}$$

We can rewrite this to introduce the chain spacing:

$$L = \sum aL_i$$

Where

$$L_i = \frac{1}{2}\frac{m}{a}\dot{\eta}_i^2 - \frac{1}{2}ka\left(\frac{\eta_{i+1} - \eta_i}{a}\right)^2$$

We now want to relate the quantity $ka$ to the Young's modulus of the material, $Y$. To do this, we first note that for an elastic rod, from Hooke's Law, the force is equal to the Young's modulus times $\xi$, the extension per unit length:

$$F = Y\xi$$

Let us apply this to our system. Consider a constant force being applied to one end of the rod. In this case, we have a uniform tension being applied to the springs, which is given by Hooke's Law for a spring:

$$F = k\left(\eta_{i+1} - \eta_i\right)$$

We can rewrite this:

$$F = ka\left(\frac{\eta_{i+1} - \eta_i}{a}\right)$$

Now recall that $a$ is the chain spacing, and therefore $ka$ is the Young's modulus, and the remaining term is exactly the displacement per unit length.

Now let us take the continuum limit of our discrete system. To do this, we move from the discrete index $i$ to a continuous index $x$. When we make this replacement, we have that $\eta_i$ becomes $\eta\left(x\right)$, and $\eta_{i+1}$ becomes $\eta\left(x+a\right)$. Previously, we labelled each mass by its counted number. Instead, we now label each mass by its location at equilibrium. $\eta\left(x\right)$ is the displacement of the mass that, when the system is in equilibrium, would be sitting at location $x$. Note that $x$ is not a dynamical variable, it is just a constant that labels the equilibrium locations, $\eta\left(x\right)$ is the dynamical variable. This is essentially downgrading $x$ to the level of $t$, instead of a dynamical variable, it is a parameter that the actual dynamical variables depend on, which is foreshadowing the introduction of relativity, but everything here is completely classical.

Now if we look at how our expressions change when we make this continuum limit:

$$\frac{\eta_{i+1} - \eta_i}{a} \rightarrow \frac{\eta\left(x+a\right) - \eta\left(x\right)}{a}$$

Now we note that in the continuum limit, this becomes $d\eta/dx$:

$$\frac{\eta\left(x+a\right) - \eta\left(x\right)}{a} = \frac{d\eta}{dx}$$

Now if we look at our summation in the continuum limit:

$$a\sum_i \rightarrow \int dx$$

And at our $m/a$, which now becomes the mass per unit length, $\mu$:

$$\frac{m}{a} \rightarrow \mu$$

Putting all of these together, we find that the full continuum Lagrangian is given by

$$L = \frac{1}{2}\int \mathrm{d}x \left[\mu\dot{\eta}^2 - Y\left(\frac{\partial\eta}{\partial x}\right)^2\right]$$

Now using the Lagrangian, we can obtain the equation of motion. Let us first look at the discrete equations of motion for the $i$th mass:

$$m\ddot{\eta}_i - k\left(\eta_{i+1} - \eta_i\right) - k\left(\eta_i - \eta_{i-1}\right) = 0$$

Suppose we now take the continuum limit of this equation. In this case, we have that:

$$\eta_{i+1} - \eta_i \to a \left(\frac{\partial \eta}{\partial x}\right)\bigg|_x$$
$$\eta_i - \eta_{i-1} \to a \left(\frac{\partial \eta}{\partial x}\right)\bigg|_{x-a}$$

This gives us the continuum expression:

$$a\left[\mu\frac{\partial^2\eta}{\partial t^2} - ka\frac{\partial^2\eta}{\partial x^2}\right] = 0$$

Now recall that $Y = ka$, so we have the continuum equation of motion:

$$\mu\frac{\partial^2\eta}{\partial t^2} - Y\frac{\partial^2\eta}{\partial x^2} = 0$$

Which is the wave equation, and our wave velocity will be $v = \sqrt{Y/\mu}$. We obtained this by taking the continuum limit of the discrete equation of motion, but let us now recover this directly from the continuum Lagrangian that we derived earlier, rather than first discussing the discrete case.

## 2.2 Continuous Lagrangian Formalism

Usually, when we do particle mechanics, we write down an action, which is the time integral of a Lagrangian. In this case our Lagrangian is itself an integral over a variable. We denote the integrand as the Lagrangian density, $\mathcal{L}$:

$$L = \frac{1}{2}\int \mathrm{d}x \left[\mu\dot{\eta}^2 - Y\left(\frac{\partial\eta}{\partial x}\right)^2\right]$$
$$\mathcal{L} = \frac{1}{2}\left[\mu\dot{\eta}^2 - Y\left(\frac{\partial\eta}{\partial x}\right)^2\right]$$

Using this denotation, the action is the time integral and the spatial integral of $\mathcal{L}$.

We want to obtain the equation of motion directly from $\mathcal{L}$. In general, the Lagrangian density is a function of $\eta$ and it its partials[1], along with the parameters that we have, $x$ and $t$:

$$\mathcal{L} = \mathcal{L}\left(\eta, \frac{\partial\eta}{\partial x}, \frac{\partial\eta}{\partial t}, x, t\right)$$

Starting from this, we define the action[2]:

$$S = \int_{t_1}^{t_2}\int_{x_1}^{x_2} \mathrm{d}x\,\mathrm{d}t\,\mathcal{L}$$

We want to extremize the action with respect to variations of the dynamical variable, $\eta$. Note that we fix the endpoints in $t$ and $x$, at both ends of the trajectory. We thus fix the variation of $\eta$ at the endpoints to be zero.

[1] Note that we are not technically restricted to just the first order partials, but for higher order partials, we end up with differential equations that are harder to solve and produce spurious solutions.

[2] Chacko uses $I$ to denote the action.

Suppose the variation is of the form:

$$\eta(x,t) = \eta_0(x,t) + \delta\eta(x,t)$$

In this form, our previous fixing of the variation is written as:

$$\begin{aligned}\delta\eta(x_1,t) &= \delta\eta(x_2,t) = 0\\ \delta\eta(x,t_1) &= \delta\eta(x,t_2) = 0\end{aligned}$$

We can now write out the variation in the action:

$$\delta S = \iint \mathrm{d}x\,\mathrm{d}t\,\left[\frac{\partial\mathcal{L}}{\partial\eta}\delta\eta + \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial x}\right)}\delta\left(\frac{\partial\eta}{\partial x}\right) + \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial t}\right)}\delta\left(\frac{\partial\eta}{\partial t}\right)\right]$$

Now thinking back to Lagrangian dynamics, we note that

$$\begin{aligned}\delta\left(\frac{\partial\eta}{\partial x}\right) &= \frac{\partial(\eta_0+\delta\eta)}{\partial x} - \frac{\partial\eta_0}{\partial x}\\ &= \frac{\partial}{\partial x}\delta\eta\end{aligned}$$

And similarly for $\frac{\partial\eta}{\partial t}$. This allows us to rewrite the change in our action:

$$\delta S = \iint \mathrm{d}x\,\mathrm{d}t\,\left[\frac{\partial\mathcal{L}}{\partial\eta}\delta\eta + \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial x}\right)}\underbrace{\delta\left(\frac{\partial\eta}{\partial x}\right)}_{\frac{\partial}{\partial x}\delta\eta} + \frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial t}\right)}\underbrace{\delta\left(\frac{\partial\eta}{\partial t}\right)}_{\frac{\partial}{\partial t}\delta\eta}\right]$$

Now integrating by parts, and noting that the boundary terms vanish because of the fixed boundary conditions:

$$\delta S = \iint \mathrm{d}x\,\mathrm{d}t\,\left[\frac{\partial\mathcal{L}}{\partial\eta} - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial x}\right)}\right) - \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial t}\right)}\right)\right]\delta\eta$$

If we set $\delta S = 0$, then we see that the only way for this to be true is if everything in the square brackets is zero, which is the same as the usual Lagrangian argument. This leaves us with the Euler-Lagrange equation for the continuous case:

$$\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial t}\right)}\right) + \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\eta}{\partial x}\right)}\right) - \frac{\partial\mathcal{L}}{\partial\eta} = 0$$

This is the equation that must be satisfied on the classical trajectory, the one that extremizes the action. Note that in the discrete case, we had a set of coupled ODEs, but in the continuous case we have a single PDE.

Let us apply this to our elastic rod, and see if this recovers the previously obtained equation of motion. We have our Lagrangian density:

$$\mathcal{L} = \frac{1}{2}\mu\left(\frac{\partial\eta}{\partial t}\right)^2 - \frac{1}{2}Y\left(\frac{\partial\eta}{\partial x}\right)^2$$

Now computing our partials:

$$\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \eta}{\partial x}\right)} = -Y\frac{\partial \eta}{\partial x}$$
$$\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \eta}{\partial t}\right)} = \mu\frac{\partial \eta}{\partial t}$$

Similarly, we can look at $\frac{\partial \mathcal{L}}{\partial \eta}$ :

$$\frac{\partial \mathcal{L}}{\partial \eta} = 0$$

Which, when inserted into our equation, gives us:

$$\mu\frac{\partial^2 \eta}{\partial t^2} - Y\frac{\partial^2 \eta}{\partial x^2} = 0$$

Which is exactly what we obtained from taking the discrete system to the continuum limit.

In this case, we have only used a single dynamical field, $\eta$. How do we generalize this to multiple fields?

Suppose we are now working with more spatial dimensions. In this case, we move from $t, x$ to $x^\mu$, where $\mu$ is an index, $\mu = 0, 1, 2, 3$, where $x^0 = t$, $x^1 = x$, $x^2 = y$, and $x^3 = z$. Suppose we have a general number of fields, so $\eta$ becomes $\eta^\rho$, where $\rho$ indexes over some arbitrary number of indices, it may be a Lorentz index, or it could be any number of scalar fields. We keep this arbitrary so that we can derive all cases at once.

We can write down the general Lagrangian density:

$$\mathcal{L} = \mathcal{L}\left(\eta^\rho, \partial_\nu \eta^\rho, x^\nu\right)$$

We want to extremize the action, which is now an integral over all spacetime:

$$S = \int \mathrm{d}^4 x\, \mathcal{L}$$

Note that in this formalism, space and time are on equal footing, so it will be easy to generalize to relativity.

Now looking at variations in $\eta^\rho$:

$$\eta^\rho = {\eta_0}^\rho + \delta\eta^\rho$$

We again fix the endpoints, $\delta\eta^\rho = 0$ at the endpoints in spacetime.

We can look at variations in the action, where we use Einstein notation, summation over repeated indices is implied:

$$\delta S = \int \mathrm{d}^4 x \left[\frac{\partial \mathcal{L}}{\partial \eta^\rho}\delta\eta^\rho + \frac{\partial \mathcal{L}}{\partial\left(\partial_\nu \eta^\rho\right)}\delta\left(\partial_\nu \eta^\rho\right)\right]$$

Again noting that $\delta\left(\partial_n u\eta^\rho\right) = \partial_\nu\left(\delta\eta^\rho\right)$, and integrating by parts, we have that

$$\delta S = \int \mathrm{d}^4x\, \left[\frac{\partial\mathcal{L}}{\partial\eta^\rho}\delta\eta^\rho - \partial_\nu\left(\frac{\partial\mathcal{L}}{\partial\left(\partial_\nu\eta^\rho\right)}\right)\right]$$

Setting this equal to zero, and using the same argument as the single field case, we have the general Euler-Lagrange equation in the continuous formalism:

$$\partial_\nu\left(\frac{\partial\mathcal{L}}{\partial\left(\partial_\nu\eta^\rho\right)}\right) - \frac{\partial\mathcal{L}}{\partial\eta^\rho} = 0$$

With this, we can take a very general Lagrangian density, and then obtain the equation of motion.

Recall the classical dynamics of a single point particle. In this case, we have the Euler-Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

We see that this is very similar to our continuous result, we just make space take the same footing as time, and we recover the same form.

## 2.3 Energy-Momentum Tensor

Recall from point particle mechanics, that we have energy conservation if the Lagrangian does not explicitly depend on time. In our continuous formalism, we will show that if the Lagrangian density does not depend on $x^0$, we have energy conservation, and if the density does not depend on $x^i$ then $p^i$ is conserved.

Let us first recall the classical proof of this, which we will then generalize to the field formalism.

If we have no explicit dependence of $L$ on $t$, then we have that

$$L = L\left(q_i, \dot{q}_i\right)$$

If this is the case, then

$$\begin{aligned}\frac{dL}{dt} &= \frac{\partial\mathcal{L}}{\partial\dot{q}_i}\frac{d}{dt}\left(\dot{q}_i\right) + \frac{\partial L}{\partial q_i}\frac{dq_i}{dt}\\ &= \frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i\right) - \dot{q}_i\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}_i}\right) + \frac{\partial L}{\partial q_i}\frac{dq_i}{dt}\end{aligned}$$

Where we have rewritten the first term. Now applying the equation of motion, we know that

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}_i}\right) = \frac{\partial L}{\partial q_i}$$

Inserting this, we see that the second and third terms cancel:

$$\frac{dL}{dt} = \frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}_i}\dot{q}_i\right)$$

Which can be rewritten:

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

Now nothing that this is just the time derivative of the Hamiltonian:

$$\frac{d}{dt}H = 0$$

We see that the total energy (the Hamiltonian) is a constant of the motion.

Now let us generalize this to the field formalism. We have a Lagrangian density, which is a function of our fields $\eta^\rho$, their partials, $\partial_\nu \eta^\rho$, but explicitly not a function of $x^\mu$:

$$\mathcal{L} = \mathcal{L}\left(\eta^\rho, \partial_\nu \eta^\rho\right)$$

We can look at $\frac{\partial L}{\partial x^\nu}$ :

$$\frac{\partial \mathcal{L}}{\partial x^\nu} = \frac{\partial \mathcal{L}}{\partial \eta^\rho}\partial_\nu \eta^\rho + \frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\partial_\nu\left(\partial_\alpha \eta^\rho\right)$$

Now rewriting the second term, just as we did in the classical derivation:

$$\frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\partial_\nu\partial_\alpha \eta^\rho = \partial_\alpha\left[\frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\partial_\nu \eta^\rho\right] - \partial_\alpha\left[\frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\right]\partial_\nu \eta^\rho$$

By the equation of motion, we see that the second term here cancels with the first term in the equation above.

Thus we are left with

$$\frac{\partial \mathcal{L}}{\partial x^\nu} = \partial_\alpha\left[\frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\partial_\nu \eta^\rho\right]$$

Which we can rewrite as:

$$\partial_\alpha\left[\frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\partial_\nu \eta^\rho - \mathcal{L}\delta^\alpha{}_\nu\right] = 0$$

We define the quantity in brackets as $T^\alpha{}_\nu$, which is known as the energy-momentum tensor (or the stress-energy tensor):

$$T^\alpha{}_\nu = \frac{\partial \mathcal{L}}{\partial\left(\partial_\alpha \eta^\rho\right)}\partial_\nu \eta^\rho - \mathcal{L}\delta^\alpha{}_\nu$$

Our equation tells us that this tensor is a constant of the motion:

$$\partial_\alpha T^\alpha{}_\nu = 0$$

We can compare this to the continuity equation from electromagnetism:

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{J}$$

Which can be rewritten in tensor notation:

$$\partial_\mu j^\mu = 0$$

Where $j^0 = \rho$, and $j^i = \boldsymbol{j}$. This equation looks very similar, except for the fact that our recently derived equation has two indices, rather than 1. The continuity equation tells us that the net current inflow is equal to the charge enclosed in the region. We can show this by integrating the equation over some region:

$$\begin{aligned}\int d^3x \, \frac{\partial \rho}{\partial t} &= \int d^3x \, (-\boldsymbol{\nabla} \cdot \boldsymbol{J}) \\ \frac{\partial}{\partial t} \int d^3x \, \rho &= -\int d^3x \, \boldsymbol{\nabla} \cdot \boldsymbol{J} \\ \frac{\partial}{\partial t} Q_{\text{enclosed}} &= -\int d\boldsymbol{A} \cdot \boldsymbol{J}\end{aligned}$$

We see that this equates the change in enclosed charge to the flux of the current flowing out of the region. In the case where the volume is all of space, current vanishes at the boundary, and we have global conservation of charge:

$$\frac{\partial}{\partial t} Q_{\text{enclosed}} = 0$$

We will show that the energy-momentum tensor relation that we derived behaves exactly the same, but with 4 independent relations, due to the extra index. In the case where $\nu = 0$, we get energy conservation, and when $\nu = 1, 2, 3$, we get momentum conservation in the respective direction. If we look at some volume, we get similar continuity relations for energy and momentum. Let us show this. We can write out the relation and then integrate over a volume:

$$\begin{aligned}\partial_t T^0{}_\nu + \partial_j T^j{}_\nu &= 0 \\ \partial_t \int d^3x \, T^0{}_\nu + \int d^3x \, \partial_j T^j{}_\nu &= 0\end{aligned}$$

If we integrate over all of space, then the second term becomes a surface integral, and vanishes:

$$\int d^3x \, \partial_j T^j{}_\nu \to \int ds \, n_j T^j{}_\nu = 0$$

Then we have just the first term:

$$\partial_t \underbrace{\int d^3x \, T^0{}_\nu}_{R_\nu} = 0$$

We denote the 4 quantities $R_\nu$ the "conserved charges". We denote $T^0{}_\nu$ as the "charge densities", and $T^j{}_\nu$ are the "charge current densities". These are all named via direct analogy to electromagnetism. We have shown that these quantities are conserved, but we have not brought in any ideas of energy or momentum.

Let us consider again the elastic rod. In this case, we can compute $T^0{}_0$:

$$T^0{}_0 = \frac{1}{2}\mu \left(\frac{\partial \eta}{\partial t}\right)^2 + \frac{1}{2} Y \left(\frac{\partial \eta}{\partial x}\right)^2$$

We see that these are the kinetic energy density and potential energy density, respectively. Thus $T^0{}_0$ is the total energy density of the system. Thus we see that the conservation of $R_0$ over all of space indicates that energy is conserved over all of space.

We could also consider ${T^j}_0$, which are energy current densities[3]. Instead, let us come to ${T^0}_x$ in the case of the elastic rod:

$$
{T^0}_x = \mu\dot{\eta}\frac{\partial\eta}{\partial x}
$$

Let us consider the momentum density of the elastic rod. There is a contribution $\mu\dot{\eta}$ (mass times velocity), which is there even for rigid body motion. We want the contribution to the momentum from wave motion inside the rod. We first notice that when wave motion happens, there is a net change in the mass of the element of the rod between $x$ and $x + dx$. If $\eta(x) > \eta(x + dx)$, then the mass between the two points has decreased. This change is given by:

$$
\mu\left[\eta(x) - \eta(x + dx)\right] \to -\mu\frac{\partial\eta}{\partial x}\,dx
$$

Where we have taken the continuum limit. The net change in momentum between $x$ and $x + dx$ associated with this motion is:

$$
\left(-\mu\frac{\partial\eta}{\partial x}\,dx\right)\dot{\eta} = \left(-\mu\dot{\eta}\frac{\partial\eta}{\partial x}\right)\,dx
$$

Which matches exactly what we got for ${T^0}_x$ (with a minus sign). This is known as the wave (or field) momentum density, and the integral of this over all space is conserved. Thus we have connected our conserved $R_\nu$ quantities to the conservation of energy and wave momentum in the elastic rod case.

## 2.4 Hamiltonian Formulation

Up until now, we have been working with the Lagrangian formalism, but at various points we will consider the Hamiltonian formulation. Let us once again consider the discrete chain of masses and springs. Conjugate to each $\eta_i$, we have a canonical momentum, $p_i$:

$$
\begin{aligned}
p_i &= \frac{\partial L}{\partial\dot{\eta}_i} \\
&= a\frac{\partial L_i}{\partial\dot{\eta}_i}
\end{aligned}
$$

When we take the continuum limit of this, we see that $p_i$ vanishes, since $L_i \sim \frac{1}{2}\mu\dot{\eta}_i^2$, and $a \to 0$. The derivative is finite, but $a$ goes to zero, so $p_i = 0$. However, we can define the momentum density $\pi$, which is nonzero in the continuum limit:

$$
\begin{aligned}
\pi &= \lim_{a\to 0}\frac{p_i}{a} \\
&= \frac{\partial\mathcal{L}}{\partial\dot{\eta}}
\end{aligned}
$$

Note that in general, $\pi$ is a function of $x$. Now that we have the conjugate momentum, we can write down the Hamiltonian:

$$
H = \sum_i p_i\dot{\eta}_i - L
$$

[3]Goldstein shows these in the case of the elastic rod, and discusses the physical intuition for them, as well as the momentum current densities.

$$= a\sum_i \left(\frac{\partial L_i}{\partial \dot{\eta}_i}\dot{\eta}_i - L_i\right)$$

Writing this in the continuum limit:

$$H = \int dx\ \left(\pi\left(x\right)\dot{\eta}\left(x\right) - \mathcal{L}\right)$$

Which defines the Hamiltonian density, $\mathcal{H}$ :

$$\mathcal{H} = \pi\left(x\right)\dot{\eta}\left(x\right) - \mathcal{L}$$

Essentially, when we define a valid continuum momentum, the Hamiltonian density is exactly what we would expect. We can generalize this to more than 1 field, where we now have multiple momenta:

$$\pi_\rho = \frac{\partial \mathcal{L}}{\partial\left(\dot{\eta}^\rho\right)}$$

For each field, we have a conjugate momentum. We can then write the multiple-field Hamiltonian density:

$$\mathcal{H} = \sum_\rho \pi_\rho \dot{\eta}^\rho - \mathcal{L}$$

Note that this is exactly what we found for ${T^0}_0$:

$$\mathcal{H} = {T^0}_0$$

This should not be very surprising, since this is exactly the same result we find in classical mechanics, as long as our Lagrangian is not explicitly time-dependent, the Hamiltonian is a constant of the motion.

## 2.5 Noether's Theorem

Let us now discuss Noether's theorem, which is a connection between the symmetry properties of the Lagrangian, and conserved quantities, known as currents. We have seen this theorem from classical mechanics, let us now discuss the form that this theorem takes in classical field theory.

**Symmetry in Physics**

For some historical background, at the turn of the 20th century, we had several revolutionary ideas. The first of these was special relativity, which not only introduced a new set of physical laws, but also changed the way that physicists do physics. When Maxwell's equations were written down, these laws came out of a lot of experimentation, a long series of experiments. The way that Einstein derived $E = mc^2$ was to realize that Maxwell's equations have a symmetry property, they are invariant under Lorentz transformations. He then imposed the requirement of Lorentz symmetry onto the other laws of physics and explored what happened. He was the first physicist to put symmetry first. After Einstein did this, Dirac required that the laws of quantum mechanics be invariant under Lorentz transformations, and derived the existence of the positron. Pauli predicted the neutrino via the symmetry of beta decays, Gell-Mann generalized isospin symmetry to discover the $\Omega^-$. This method was used extensively since Einstein in the 20th century, the application of symmetries to the laws of physics.

**Theorem 2.1.** *Noether's Theorem. For every continuous symmetry transformation of the Lagrangian, there exists a conserved current.*

Note that this is only in one direction, symmetries imply conserved quantities, but conserved quantities do not imply symmetries. Another thing to note is that the transformations that produce conserved currents are necessarily continuous, there must be some infinitesimal generator of the symmetry transformation.

Let us now prove Noether's Theorem. Let us first consider a transformation[4]:

$$x^\mu \to x^{\mu'} = x^\mu + \delta x^\mu \left(x^\nu\right)$$

Where the second term is a function $x^\mu$ of $x^\nu$. This can be any general transformation. This transformations affects our field:

$$\eta^\rho \left(x^\mu\right) \to \eta^{\rho'} \left(x^{\mu'}\right) = \eta^\rho \left(x^\mu\right) + \delta\eta^\rho \left(x^\mu\right)$$

This changes our Lagrangian density, but we can claim that the functional form is the same if the transformation is a symmetry of the Lagrangian:

$$\mathcal{L}\left[\eta^\rho\left(x^\mu\right), \partial_\nu \eta^\rho\left(x^\mu\right), x^\mu\right] = \mathcal{L}\left[\eta^{\rho'}\left(x^{\mu'}\right), \partial'_\nu \eta^{\rho'}\left(x^{\mu'}\right), x^{\mu'}\right] \tag{1}$$

This is known as *form invariance*, the form of the Lagrangian does not change. If the transformation is not a symmetry, it would be $\mathcal{L}'$ on the right side, rather than the original $\mathcal{L}$. The other claim that we could make is that the action remains the same:

$$S' = \int_{\Omega'} dx^{\mu'}\, \mathcal{L}'\left[\eta^\rho\left(x^{\mu'}\right), \partial'_\nu \eta^{\rho'}\left(x^{\mu'}\right), x^{\mu'}\right] = \int_\Omega dx^\mu\, \mathcal{L}\left[\eta^\rho\left(x^\mu\right), \partial_\nu \eta^\rho\left(x^\mu\right), x^\mu\right] \tag{2}$$

This is known as *scale invariance*. Note that the Jacobian determinant in the left integral is not present, this is what makes the transformation a symmetry. If we had explicitly written out the Jacobian determinant then this statement would be true for all transformations. According to Goldstein, a transformation must require both of these invariances for the transformation to be a symmetry. However, according to Chacko, there is a weaker claim that still holds. Consider the case where form invariance is not met, but scale invariance is. The argument for this case existing is that a scaling transformation might change $d^4x$, but the functional form of the Lagrangian might be changed in the exact opposite way, in order to keep the action integral invariant. Thus we would not have the exact same functional form of the Lagrangian, breaking form invariance, but the action would be invariant, giving us scale invariance. However, let us just go with what Goldstein says, because the most common case is that both conditions are met.

Let us do an example of a transformation and Lagrangian. Consider the Lagrangian:

$$\mathcal{L} = \partial_\mu \phi^\dagger \partial^\mu \phi - m^2 \phi^\dagger \phi + m^2 \left(\phi^2 + \phi^{\dagger 2}\right)$$

This is a scalar field, the dagger represents complex conjugation. Now consider a field

[4]Note that this is a *passive* transformation, but can be done in the language of active transformations as well.

transformtaion:

$$\phi \to \phi' = e^{i\alpha}\phi$$

In this case, we can look at $\phi'^{\dagger}$:

$$\phi'^{\dagger} = e^{-i\alpha}\phi^{\dagger}$$

With this, we can rewrite our Lagrangian density in terms of $\phi'$ and $\phi'^{\dagger}$:

$$\begin{aligned}
\mathcal{L}' &= \partial_\mu \left[e^{i\alpha}\phi'^{\dagger}\right] \partial^\mu \left[e^{-i\alpha}\phi'\right] - m^2 \left[e^{i\alpha}\phi'^{\dagger}\right] \left[e^{-i\alpha}\phi'\right] + m^2 \left(e^{-2i\alpha}\phi'^2 + e^{2i\alpha}\phi'^{\dagger 2}\right) \\
&= \partial_\mu \phi'^{\dagger}\partial^\mu \phi' - m^2 \phi'^{\dagger}\phi' + m^2 \left(e^{-2i\alpha}\phi'^2 + e^{2i\alpha}\phi'^{\dagger 2}\right)
\end{aligned}$$

We see that this transformation is not a symmetry transformation, since we have an extra $e^{\pm 2i\alpha}$ in the third term. If we removed the last term from the Lagrangian, then this would be a symmetry transformation of the modified Lagrangian, since the first two terms remain form invariant.

Let us now continue proving Noether's theorem. Suppose we satisfy both Defn. 1 and Defn. 2, we have both form and scale invariance. In this case, the statement of scale invariance can be rewritten as:

$$\int_{\Omega'} dx^\mu\, \mathcal{L}\left[\eta^{\rho'}(x^\mu), \partial_\nu \eta^{\rho'}(x^\mu), x^\mu\right] - \int_{\Omega} dx^\mu\, \mathcal{L}\left[\eta^{\rho}(x^\mu), \partial_\nu \eta^{\rho}(x^\mu), x^\mu\right] = 0$$

Where we have changed the Lagrangian in the left integral to $\mathcal{L}$, via form invariance. Note that we have also changed the dummy variable of integration of the left integral from $x'$ to $x$. These integrals differ in their region of integration, as well as the fields that are in the Lagrangian. In other words, we have an of $\Delta\mathcal{L}$ over the region $\Omega$, and we have an integral of $\mathcal{L}$ over the region $\Omega' - \Omega$. Thus we can rewrite the equation as:

$$\underbrace{\int_{\Omega} dx^\mu \left(\mathcal{L}\left[\eta^{\rho'}, \partial_\nu \eta^{\rho'}, x^\mu\right] - \mathcal{L}\left[\eta^{\rho}, \partial_\nu \eta^{\rho}, x^\mu\right]\right)}_{\Delta\mathcal{L} \text{ in } \Omega} + \underbrace{\int_{\Omega'-\Omega} dx^\mu\, \mathcal{L}\left[\eta^{\rho'}, \partial_\nu \eta^{\rho'}, x^\mu\right]}_{\mathcal{L} \text{ in disjoint region}} = 0 \tag{3}$$

The first integral seems workable, but what do we do with the second integral? We will not treat this integral honestly, instead we will deal with it in 1 dimension and then claim that it generalizes to the 4D integral. Consider the analogous 1D case of our equation:

$$\begin{aligned}
\int_{a+\delta a}^{b+\delta b} dx\, \left[f(x) + \delta f(x)\right] - \int_a^b dx\, f(x) &= 0 \\
\int_a^b dx\, \delta f(x) + \int_b^{b+\delta b} dx\, \left[f(x) + \delta f(x)\right] - \int_a^{a+\delta a} dx\, \left[f(x) + \delta f(x)\right] &= 0
\end{aligned}$$

Now dropping the $\delta f(x)$ in the integrals that are over infinitesimal regions, and claiming that $f(x)$ is approximately constant over such small regions:

$$\begin{aligned}
\int_a^b dx\, \delta f(x) + \int_b^{b+\delta b} dx\, \left[f(x) + \delta f(x)\right] - \int_a^{a+\delta a} dx\, \left[f(x) + \delta f(x)\right] &= 0 \\
\int_a^b dx\, \delta f(x) + f(b)\,\delta b - f(a)\,\delta a &= 0
\end{aligned}$$

Now rewriting this to "undo" an integration:

$$\int_a^b dx \left(\delta f(x) + \frac{d}{dx}\left[f(x)\,\delta x\right]\right) = 0$$

Where $\delta x$ is any smooth function of $x$ that satisfies the boundary conditions of the integral. Now what is the higher dimensional analog of our newly derived 1D equation? We claim that it is:

$$\int_{\Omega'-\Omega} dx^\mu\, \mathcal{L}\left[\eta^{\rho'}, \partial_\nu \eta^{\rho'}, x^\mu\right] = \int_S dS_\mu\, \mathcal{L}\left[\eta^\rho, \partial_\nu\eta^\rho, x^\mu\right]\delta x^\mu$$

Where the term on the right is the result of the integral over the infinitesimal disjoint region. Similarly to the 1D case, we can write this as a total derivative:

$$\int_S dS^\mu\, \mathcal{L}\left[\eta^\rho, \partial_\nu\eta^\rho, x\right]\delta x_\mu = \int_\Omega dx^\nu \frac{\partial}{\partial x^\nu}\left[\mathcal{L}\left[\eta^\rho, \partial_\nu\eta^\rho, x^\mu\right]\delta x^\mu\right]$$

This is essentially Gauss's Law in 3+1 dimensions. We are saying that the Lagrangian does not have enough time to change over the small disjoint region, and we can integrate it over the surface of the disjoint region. Now let us return to Equation 3, where we have now dealt with the second integral. Let us now consider the first term. We can rewrite this as:

$$\int_\Omega dx^\mu \left(\mathcal{L}\left[\eta^{\rho'}, \partial_\nu\eta^{\rho'}, x^\mu\right] - \mathcal{L}\left[\eta^\rho, \partial_\nu\eta^\rho, x^\mu\right]\right) = \int_\Omega dx^\mu \left[\frac{\partial\mathcal{L}}{\partial\eta^\rho}\bar{\delta}\eta^\rho + \frac{\partial\mathcal{L}}{\partial\left(\partial_\nu\eta^\rho\right)}\bar{\delta}\left(\partial_\nu\eta^\rho\right)\right]$$

Where $\bar{\delta}\eta$ is the change in $\eta$ at the point with coordinates $x^\mu$ (as opposed to $\delta\eta$, which is the change in $\eta$ at the same physical point). To demonstrate the difference between our two deltas, consider a field $\phi(x)$, which is a scalar under rotations. We take some physical point $x$, and we rotate our coordinate system, and the new coordinate of the same physical point is now $x'$. The field at the physical point must always be the same, regardless of the coordinate system:

$$\phi(x) = \phi'\left(x'\right)$$

Knowing this, we can find $\phi'$:

$$\begin{aligned}\phi(x) &= \phi'\left(x'\right)\\ \phi(x) &= \phi'\left(R^{-1}x\right)\end{aligned}$$

Recall that

$$\eta^{\rho'}\left(x^{\mu'}\right) = \eta^\rho\left(x^\mu\right) + \delta\eta^\rho\left(x^\mu\right)$$

For a scalar under rotations, the value at the same physical point does not change, so $\delta\eta^\rho\left(x^\mu\right) = 0$. However, there is a point in our new coordinate system that has the same label as our physical point in the original coordinates. This is a *different* physical point, but they have the same coordinates. This is how we define $\bar{\delta}\eta^\rho$:

$$\bar{\delta}\eta^\rho = \eta^{\rho'}(x) - \eta^\rho(x)$$

Note that for our scalar field, this is *not* zero, unlike $\delta\eta^\rho$. We can write out what $\bar{\delta}\eta^\rho$ is:

$$\bar{\delta}\eta^\rho = \eta^{\rho'}(x) - \eta^\rho(x)$$

$$
\begin{aligned}
&= \eta^{\rho'}\left(x' - \delta x\right) - \eta^{\rho}\left(x\right) \\
&= \eta^{\rho'}\left(x'\right) - \delta x^{\alpha}\frac{\partial \eta^{\rho'}}{\partial x'^{\alpha}} - \eta^{\rho}\left(x\right) \\
&= -\delta x^{\alpha}\frac{\partial \eta^{\rho}}{\partial x^{\alpha}}
\end{aligned}
$$

Note that we drop the primes in the derivative because we already have a $\delta x$, the difference between the primed and unprimed coordinates is subleading relative to $\delta x$. We can now compute $\bar{\delta}\left(\partial_\nu \eta^\rho\right)$ via analogy to $\bar{\delta}\eta^\rho$:

$$
\begin{aligned}
\bar{\delta}\left(\partial_\nu \eta^\rho\right) &= \partial_\nu \eta^{\rho'}\left(x\right) - \partial_\nu \eta^{\rho}\left(x\right) \\
&= \partial_\nu\left[\bar{\delta}\eta^\rho\left(x\right)\right]
\end{aligned}
$$

With these two quantities computed, we now look at the integral we had, and we can replace the $\frac{\partial \mathcal{L}}{\partial \eta^\rho}$ using the equations of motion:

$$
\int_\Omega dx^\mu \left[\frac{\partial \mathcal{L}}{\partial \eta^\rho}\bar{\delta}\eta^\rho + \frac{\partial \mathcal{L}}{\partial\left(\partial_\nu \eta^\rho\right)}\bar{\delta}\left(\partial_\nu \eta^\rho\right)\right] = \int_\Omega dx^\mu \left[\frac{\partial}{\partial x^\nu}\left(\frac{\partial \mathcal{L}}{\partial\left(\partial_\nu \eta^\rho\right)}\bar{\delta}\eta^\rho\right)\right]
$$

Now recombining this term with the disjoint integral term:

$$
\int_\Omega dx^\mu \frac{\partial}{\partial x^\nu}\left[\frac{\partial \mathcal{L}}{\partial\left(\partial_\nu \eta^\rho\right)}\bar{\delta}\eta^\rho + \mathcal{L}\delta x^\mu\right] = 0
$$

Now we recall that we never specified what $\Omega$ was, it can be any 4-volume. Thus the integrand must vanish for all volumes, and therefore the quantity in the total derivative must be constant. This is denoted $j$:

$$
j^\nu = \frac{\partial \mathcal{L}}{\partial\left(\partial_\nu \eta^\rho\right)}\bar{\delta}\eta^\rho + \mathcal{L}\delta x^\mu \tag{4}
$$

This is the Noether current, and is conserved, $\partial_\mu j^\mu = 0$.

**Noether Current Examples**

The first example we will look at is translations. Consider a Lagrangian density that is invariant under translations. In this case, the value of the field at the physical point does not change, regadless of whether it is a scalar field or a vector field. Thus we have that

$$
\eta^{\rho'}\left(x'\right) = \eta^\rho\left(x\right)
$$

Which gives us that $\delta\eta^\rho\left(x\right) = 0$. We can explicitly define our translation:

$$
x'^{\nu} = x^\nu + a^\nu
$$

and so $\delta x^\nu = a^\nu$. We now want to find $\bar{\delta}\eta^\rho$:

$$
\begin{aligned}
\bar{\delta}\eta^\rho &= \eta^{\rho'}\left(x\right) - \eta^\rho\left(x\right) \\
&= -a^\nu \partial_\nu \eta^\rho
\end{aligned}
$$

From this, we can write out the Noether current:

$$
j^\nu = \frac{\partial \mathcal{L}}{\partial\left(\partial_\nu \eta^\rho\right)}\left[-a^\alpha \partial_\alpha \eta^\rho\right] + \mathcal{L}a^\nu
$$

$$= -a^{\alpha}\underbrace{\left[\frac{\partial \mathcal{L}}{\partial\left(\partial_{\nu}\eta^{\rho}\right)}\partial_{\alpha}\eta^{\rho} - \mathcal{L}\delta^{\nu}{}_{\alpha}\right]}_{T^{\nu}{}_{\alpha}}$$

We see that we recover the energy-momentum tensor as our conserved quantity, spacetime translational invariance leads to the conservation of the energy-momentum tensor.
Let us do another example. Consider the Lagrangian density:

$$\mathcal{L} = \partial_{\mu}\phi^{\dagger}\partial^{\mu}\phi - m^2\phi^{\dagger}\phi$$

Now consider the transformation:

$$\begin{aligned}\phi &\to e^{i\alpha}\phi = \phi' \\ \phi^{\dagger} &\to e^{-i\alpha}\phi^{\dagger} = \phi'^{\dagger}\end{aligned}$$

We can first show that this is a symmetry, and then we can find the Noether current. To show that it is a symmetry, we must show form invariance:

$$\begin{aligned}\mathcal{L} &= \partial_{\mu}\left(e^{i\alpha}\phi'^{\dagger}\right)\partial^{\mu}\left(e^{-\alpha}\phi'\right) - m^2\left(e^{i\alpha\phi'^{\dagger}}e^{-i\alpha}\phi'\right) \\ &= \partial_{\mu}\phi'^{\dagger}\partial^{\mu}\phi' - m^2\phi'^{\dagger}\phi'\end{aligned}$$

We see that if we insert the transformed coordinates, we obtain the same functional form, giving us form invariance. Scale invariance in this case is trivially obtained, since the transformation does not depend on the coordinates. Thus this transformation is indeed a symmetry.
Now let us compute the Noether current. We can compute $\bar{\delta}\phi$, which, since we haven't changed the coordinates, is the same as $\delta\phi$:

$$\begin{aligned}\bar{\delta}\phi &= \phi'(x) - \phi(x) \\ &= e^{i\alpha}\phi(x) - \phi(x) \\ &= i\alpha\phi(x)\end{aligned}$$

Where we have Taylor expanded the exponential, since we consider an infinitesimal transformation. We can do the same for $\phi^{\dagger}$, and we find that

$$\bar{\delta}\phi^{\dagger} = -i\alpha\phi^{\dagger}$$

We can now insert these into the definition of the Noether current:

$$\begin{aligned}j^{\nu} &= \frac{\partial \mathcal{L}}{\partial\left(\partial_{\nu}\phi\right)}\bar{\delta}\phi + \frac{\partial \mathcal{L}}{\partial\left(\partial_{\nu}\phi^{\dagger}\right)}\bar{\delta}\phi^{\dagger} \\ &= \left(\partial^{\nu}\phi^{\dagger}\right)(i\alpha\phi) + \partial_{\nu}\phi\left(-i\alpha\phi^{\dagger}\right) \\ &= -i\alpha\left[\phi^{\dagger}\partial^{\nu}\phi - \phi\partial^{\nu}\phi^{\dagger}\right]\end{aligned}$$

# 3 Relativistic Wave Equations

*This discussion comes from two books, Sakurai's Advanced Quantum Mechanics, and Relativistic Quantum Mechanics, by Bjorken and Drell.*

Suppose we want to write down a wave equation that obeys special relativity, that is, how do we generalize the Schrödinger equation? We have an energy relation:

$$E = \frac{p^2}{2m} + V(x)$$

Which then turns into a wave equation, $E$ and $t$ become operators:

$$i\hbar\frac{\partial}{\partial t}\phi = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V\psi$$

This equation is only invariant under Galilean symmetries, not Lorentz transformations. The naive generalization is to use the relativistic energy momentum relation:

$$E = \sqrt{c^2p^2 + m^2c^4}$$

Which turns our wave equation into:

$$i\hbar\frac{\partial\psi}{\partial t} = \sqrt{-\hbar^2c^2\boldsymbol{\nabla}^2 + m^2c^4}\psi$$

How do we deal with this square root? The first idea is to square both sides of our energy momentum relation:

$$E^2 = c^2p^2 + m^2c^4$$

We can then write out the wave equation:

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = -\hbar^2c^2\boldsymbol{\nabla}^2\psi + m^2c^4\psi \tag{5}$$

This is known as the relativistic Schrödinger equation[5], but is more commonly known as the Klein-Gordon equation. Writing this equation in relativistic notation:

$$\partial_\alpha\partial^\alpha\psi + \frac{m^2c^2}{\hbar^2}\psi = 0$$

Let us look for plane wave solutions of this equation:

$$\begin{aligned}\psi(\boldsymbol{x}, t) &= e^{i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega t)} \\ &= \exp\left[\frac{\boldsymbol{p}\cdot\boldsymbol{x} - Et}{\hbar}\right]\end{aligned}$$

Where $\boldsymbol{p} = \hbar\boldsymbol{k}$ and $E = \hbar\omega$. If we insert this ansatz into our differential equation:

$$-\frac{\omega^2}{c^2} + k^2 + \left(\frac{mc}{\hbar}\right)^2 = 0$$

[5] Schrödinger actually wrote this equation down before the non-relativistic equation, but he abandoned it due to some of the issues we will see shortly.

From this, we have that

$$E = \pm\sqrt{c^2p^2 + m^2c^4}$$

Immediately, we have a problem. We see that we have negative energy solutions, which implies that we can have arbitrarily negative energies, there is an infinite number of these negative energy states! We ignore this and proceed (as physicists usually do).

In non-relativistic quantum mechanics, we have conservation of probability, does the Klein-Gordon wave equation also have this property? Looking back at the regular quantum mechanical wave equation:

$$-i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V\psi$$

Taking the complex conjugate of both sides:

$$-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi * +V\psi *$$

If we take the wave equation and multiply both sides by $\psi^*$, and subtract the product of this conjugated wave equation and $\psi$ (taking the Wronskian), we find that:

$$i\hbar\frac{\partial}{\partial t}\left(\psi\psi^*\right) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}\cdot\left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right)$$

This is a continuity equation (compare this to $\frac{\partial\rho}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{j}$ from electromagnetism). We can write this in a form that makes it more clear:

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{S} = 0$$

Where $\rho = \psi^*\psi$ is the conserved probability density. Note that $\rho$ is positive definite, which is necessary if we want to interpret $\rho$ as a probability[6]. From this continuity equation, we have that the probability over all space is a constant in time.

Now let us consider the Klein-Gordon theory. In this case, we can again take the Wronskian, after which we find:

$$\frac{1}{c^2}\frac{\partial}{\partial t}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right) = \boldsymbol{\nabla}\cdot\left(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*\right)$$

Where we have dropped factors of $\hbar$ and $c$. We see that we again find a continuity equation, with the same $\boldsymbol{S}$, but the $\rho$ is not the same:

$$\frac{\partial\tilde{\rho}}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{S} = 0$$

Here $\tilde{\rho}$ is no longer $\psi^*\psi$:

$$\tilde{\rho} = \frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right)$$

This is real, but is no longer positive definite, we cannot identify this with a probability density. People ignored this and proceeded. What finally killed the Klein-Gordon equation was the calculation of the fine structure of Hydrogen using this theory, which disagreed with experiment, and the theory was *then* abandoned as a wave equation.

What do we do now? The Klein-Gordon equation does not work as a relativistic wave equation. From this, we move to the Dirac equation.

[6] Famously, this was first done by Max Born, for which he received a Nobel Prize.

## 3.1 The Dirac Equation

Dirac looked at the Schrodinger equation and the Klein-Gordon equation, and noted that in the Schrodinger equation, we have only 1 order of time derivatives, while the Klein-Gordon equation is second order in time. So he attempted to write down an equation that was first order in time. To do this, we have to deal with the square root that we ran into earlier:

$$E = \sqrt{c^2p^2 + m^2c^4}$$

To deal with this, Dirac rewrote this as:

$$E = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + mc^2\beta$$

Where $\alpha_i$ and $\beta$ are matrices. Note that this makes the energy a matrix, and the wavefunction a column vector. To do this, if we square this, we better get the right expression:

$$\begin{aligned} E^2 &= \left(c\boldsymbol{\alpha} \cdot \boldsymbol{p} + mc^2\beta\right)^2 \\ &= \left(c\left(\alpha_x p_x + \alpha_y p_y + \alpha_z p_z\right) + mc^2\beta\right)^2 \\ &= c^2\left(\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2 + \beta^2 m^2 c^2\right) \\ &+ c^2\left[\left(\alpha_x\alpha_y + \alpha_y\alpha_x\right)p_xp_y + \left(\alpha_y\alpha_z + \alpha_z\alpha_y\right)p_yp_z + \left(\alpha_z\alpha_x + \alpha_x\alpha_z\right)p_zp_x\right] \\ &+ \left[\left(\alpha_x\beta + \beta\alpha_x\right)p_xmc^2 + \left(\alpha_y\beta + \beta\alpha_y\right)p_ymc^2 + \left(\alpha_z\beta + \beta\alpha_z\right)p_zmc^2\right] \end{aligned}$$

Now compare this mess to the correct expression:

$$E^2 = c^2p_x^2 + c^2p_y^2 + c^2p_z^2 + m^2c^4$$

To have these match, we have many conditions that must be met. The first is that

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \mathbb{I}$$

We also have an anticommutation relation:

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 0$$

for $i \neq j$. We also have that

$$\beta\alpha_i + \alpha_i\beta = 0$$

And $\beta^2 = \mathbb{I}$.

We must find 4 matrices $\{\alpha_x, \alpha_y, \alpha_z, \beta\}$ that satisfy these properties. Let us first postpone a discussion of what these matrices are. Suppose we have a set of matrices that satisfy these properties, what does our theory look like? We can write our Hamiltonian:

$$\hat{H} = c\boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} + mc^2\beta$$

If we now enforce that the Hamiltonian is Hermitian, $\hat{H} = \hat{H}^\dagger$, we have another condition on the matrices:

$$\begin{aligned} \alpha_i &= \alpha_i^\dagger \\ \beta &= \beta^\dagger \end{aligned}$$

We see we need 4 Hermitian, idempotent, and anticommuting matrices. We can then write out our wave equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -i\hbar c\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\psi + mc^2\beta\psi \tag{6}$$

We see that this is indeed first order in time, so we have a decent chance of getting a conserved positive definite probability density. Let us determine if this is indeed the case. We can take the Hermitian conjugate of our wave equation:

$$-i\hbar\frac{\partial\psi^\dagger}{\partial t} = i\hbar c\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\alpha} + mc^2\psi^\dagger\beta$$

Multiplying this by $\psi$, and then multiplying our wave equation by $\psi^\dagger$, and then subtracting the two, we find that

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left(\psi^\dagger\psi\right) &= -i\hbar c\left(\psi^\dagger\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}\psi + \boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\alpha}\psi\right) \\ &= -i\hbar c\boldsymbol{\nabla}\cdot\left(\psi^\dagger\boldsymbol{\alpha}\psi\right) \end{aligned}$$

Thus we have our probability current density $\boldsymbol{S} = c\psi^\dagger\boldsymbol{\alpha}\psi$, and our probability density $\rho = \psi^\dagger\psi$.

Up until now, we have assumed that there exists a set of 4 matrices that satisfy these properties. Let us now see if we can in fact find such a set of matrices. If we wanted a set of 3 matrices, we could use the Pauli matrices, since they satisfy these conditions. However, we need 4! In fact, if we were to work in 2+1D, we would be able to use the Pauli matrices, since we would only need a set of 3 matrices. This implies that we might be able to generalize from the Pauli matrices to something that works in 3+1D.

This leads us to the Dirac matrices. We want to find whether or not we can find four $2\times 2$ matrices that are Hermitian, mutually anticommuting, and idempotent. Since the Pauli matrices and the identity span all $2\times 2$ Hermitian matrices, we can actually prove that there is no such fourth matrix. What about $3\times 3$ matrices? We can actually prove that the Dirac matrices must be *even* dimensional, so $3\times 3$ will not work.

*Proof.* The $\alpha_i$ matrices must be Hermitian. Thus we can diagonalize one of them, via some unitary transformation. Note that $\alpha_i^2 = \mathbb{I}$ must be true before and after the diagonalization. Also note that since $\alpha_i$ is idempotent, it has eigenvalues of $\pm 1$. This argument applies to all of the 4 matrices, they all have eigenvalues $\pm 1$. Now $\alpha_i\beta + \beta\alpha_i = 0$ (one of our conditions), which implies that $\beta^{-1}\alpha_i\beta = -\alpha_i$. Now taking the trace, and applying the cyclic property of the trace, we find that

$$\mathrm{Tr}\left[\alpha_i\right] = 0$$

We have shown that the eigenvalues are $\pm 1$, and the trace is zero, so there must be an equal number of $+1$ eigenvalues and $-1$ eigenvalues, and therefore the matrix must be even dimensional. □

From this, we know that we need the Dirac matrices to be $4\times 4$ at the very least. There is no unique set of matrices, but here is one set:

$$\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix} \qquad \beta = \begin{bmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{bmatrix}$$

Where $\mathbb{I}_2$ is the $2 \times 2$ identity matrix, and $\sigma_i$ is a $2 \times 2$ Pauli matrix. Since this set is not unique, different books use different choices. Some choices work better for the relativistic limit, and others in the non-relativistic limit. Peskin for example, chooses a set that is better for relativistic computations. We can transition between different sets of these matrices by a similarity transformation:

$$\alpha_i' = S\alpha_i S^{-1} \qquad \beta' = S\beta S^{-1}$$

Where $S$ is a unitary matrix, because the $\alpha$s and $\beta$ are Hermitian.

We have now found an explicit set of matrices that satisfy our conditions, so let us look for plane wave solutions of the Dirac equation. Rewriting our equation:

$$\left(-i\hbar c\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + mc^2\beta\right)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

This is not the usual way we write the Dirac equation. This equation (as we will see) is invariant under Lorentz transformations, but this is not very clearly seen. To make this more clear, we multiply both sides by $\beta$, and divide by $c$:

$$\left(-i\hbar\beta\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + mc\right)\psi = i\hbar\frac{\beta}{c}\frac{\partial\psi}{\partial t}$$

This equation has the form

$$i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0$$

Where we define[7] $\gamma^0 = \beta$, and $\gamma^i = \beta\alpha^i$. From this, we can write the Dirac equation using natural units, where $\hbar = c = 1$:

$$\left(i\gamma^\mu\partial_\mu - m\right)\psi = 0 \tag{7}$$

In natural units, everything is now described in terms of energy (eV). Note that we will also be using Heaviside-Lorentz units[8], in which Coulomb's Law is written as

$$F_C = \frac{q_1 q_2}{4\pi r^2}$$

Heaviside-Lorentz is essentially SI units, except we don't have the $\varepsilon_0$.

We can rewrite the $\alpha$ and $\beta$ commuatation relations in terms of the $\gamma$ matrices:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$$

Now let us return to looking for plane wave solutions. We want solutions of the form:

$$\psi\left(x, t\right) = w\left(\boldsymbol{p}\right)e^{i(\boldsymbol{p}\cdot\boldsymbol{x} - Et)}$$

For the sake of simplicity, we will choose $\boldsymbol{p} = p\hat{z}$. $w$ is a four component matrix, but it is convenient to write this as a two-component object (since the $\gamma$ matrices can be separated into $2 \times 2$ block matrices):

$$w = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} = \begin{pmatrix} w_A \\ w_B \end{pmatrix}$$

[7] Note that we define $x^0 = ct$

[8] Gaussian units are easier in the case where we start with Coulomb's Law itself, but Heaviside-Lorentz is nicer when starting from the Lagrangian, which is what we will be doing. SI units are never useful.

If we insert our plane wave solution into the Dirac equation, since the derivative $\partial_\mu \psi$ is zero along the $x$ and $y$ direction, we have

$$\left(\gamma^0 - \gamma^3 p - m\right) w = 0$$

Now inserting the $\gamma$ matrices in block form:

$$\left[E\begin{pmatrix} 0 & \mathbb{I}_2 \\ \mathbb{I}_2 & 0 \end{pmatrix} - p\begin{pmatrix} 0 & \sigma_3 \\ -\sigma_3 & 0 \end{pmatrix} - m\right]\begin{pmatrix} w_A \\ w_B \end{pmatrix} = 0$$

This gives us two equations:

$$Ew_B - p\sigma_3 w_B - mw_A = 0 \tag{8}$$
$$Ew_A + p\sigma_3 w_A - mw_B = 0 \tag{9}$$

Now we can rewrite Eqn 8:

$$w_A = \frac{(E - p\sigma_3)}{m} w_B$$

Inserting this into Eqn 9:

$$\frac{(E + p\sigma_3)(E - p\sigma_3)}{m} w_B - mw_B = 0$$

Using the fact that $\sigma_3^2 = \mathbb{I}$, we are left with

$$\left(E^2 - p^2 - m^2\right) w_B = 0$$

From which we have

$$E = \pm\sqrt{p^2 + m^2}$$

Let us make a few comments about what we have seen. The first is that $w_A$ and $w_B$ are not independent, if we know one of them, we can find the other. The other thing to note is that unless the final condition on the energy (the energy dispersion relation) is satisfied, we have a trivial solution. Perhaps the most glaring issue is that we have a nontrivial negative energy solution, we were not able to avoid the issue that we first saw in the Klein-Gordon theory.

Note that $w_B$ can take two independent values:

$$w_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and since $E$ can be either positive or negative, we have a total of four independent plane wave solutions. Listing them out:

$$w_{\uparrow +}: \quad w_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad w_A = \begin{pmatrix} \frac{E_+ - p}{m} \\ 0 \end{pmatrix}$$
$$w_{\downarrow +}: \quad w_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad w_A = \begin{pmatrix} 0 \\ \frac{E_+ + p}{m} \end{pmatrix}$$
$$w_{\uparrow -}: \quad w_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad w_A = \begin{pmatrix} \frac{E_- - p}{m} \\ 0 \end{pmatrix}$$

$$w_{\downarrow -}: \quad w_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad w_A = \begin{pmatrix} 0 \\ \frac{E_- + p}{m} \end{pmatrix}$$

We label these independent solutions (for reasons that will become clear later) with spin indices, as well as the sign of the energy. These solutions are orthogonal:

$$w_{\uparrow +} \cdot w_{\uparrow -} = w_{\uparrow +} \cdot w_{\downarrow +} = \cdots = 0$$

These are generally not written in this way, people have come up with notation that allows for easier computation. We can alter the normalizations of these solutions:

$$u_1 (p): \quad w_B = \begin{pmatrix} \sqrt{E_+ + p} \\ 0 \end{pmatrix} \qquad w_A = \begin{pmatrix} \sqrt{E_+ - p} \\ 0 \end{pmatrix}$$
$$u_2 (p): \quad w_B = \begin{pmatrix} 0 \\ \sqrt{E_+ - p} \end{pmatrix} \qquad w_A = \begin{pmatrix} 0 \\ \sqrt{E_+ + p} \end{pmatrix}$$

These are the two positive energy solutions ($w_{\uparrow +}$ and $w_{\downarrow +}$). For the negative energy solutions, we use a different convention, we look for solutions of the Dirac equation of the form

$$\psi (x) = \tilde{w} (p) e^{i(Et - p\hat{z})}$$

with $E > 0$. Essentially, the negative energy solutions propagating in a certain direction can be written in the same form as *positive* energy solutions propagating in the *opposite* direction.

We can again break $\tilde{w}$ into a two-component object:

$$\tilde{w} = \begin{pmatrix} \tilde{w}_A \\ \tilde{w}_B \end{pmatrix}$$

We can then rewrite our negative energy solutions:

$$w_{\uparrow -}: \quad \tilde{w}_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \tilde{w}_A = \begin{pmatrix} -\frac{E_+ + p}{m} \\ 0 \end{pmatrix}$$
$$w_{\downarrow -}: \quad \tilde{w}_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad \tilde{w}_A = \begin{pmatrix} 0 \\ -\frac{E_+ - p}{m} \end{pmatrix}$$

We can again change the normalization, and write down the negative energy solutions:

$$v_1 (p): \quad \tilde{w}_B = \begin{pmatrix} \sqrt{E_+ + p} \\ 0 \end{pmatrix} \qquad \tilde{w}_A = \begin{pmatrix} -\sqrt{E_+ - p} \\ 0 \end{pmatrix}$$
$$v_2 (p): \quad \tilde{w}_B = \begin{pmatrix} 0 \\ \sqrt{E_+ - p} \end{pmatrix} \qquad \tilde{w}_A = \begin{pmatrix} 0 \\ -\sqrt{E_+ + p} \end{pmatrix}$$

With this new notation, we have that $u_i (p)$ represent positive energy solutions moving along $\boldsymbol{p}$, and $v_i (p)$ are negative energy solutions moving opposite $\boldsymbol{p}$.

There are certain standard properties of these solutions that are useful when doing calculations. We can begin with another definition:

$$\overline{w} = w^\dagger \gamma^0$$

For any four component object $w$. From this, we have that

$$\overline{u}^r(p)\,u^s(p) = 2m\delta^{rs}$$
$$u^{r\dagger}(p)\,u^s(p) = 2E_p\delta^{rs}$$

And for the $v$s:

$$\overline{v}^r(p)\,v^s(p) = -2m\delta^{rs}$$
$$v^{p\dagger}(p)\,v^s(p) = 2E_p\delta^{rs}$$

We also have that

$$\overline{v}^r(p)\,u^s(p) = 0$$
$$\overline{u}^r(p)\,v^s(p) = 0$$

However,

$$v^{r\dagger}(p)\,u^s(p) \neq 0$$
$$u^{r\dagger}(p)\,v^s(p) \neq 0$$

The above property arises because the $u$s and $v$s are propagating in opposite directions, so in fact:

$$v^{r\dagger}(p)\,u^s(-p) = 0$$
$$u^{r\dagger}(p)\,v^s(-p) = 0$$

We can now also write down a summation property:

$$\sum_{s=1,2} u^s(p)\,\overline{u}^s(p) = \not{p} - m$$

Where $\not{p} = p_\mu\gamma^\mu$[9]. Note that this is not an inner product, this is an outer product (column vector times a row vector), and thus we are left with a matrix, rather than a number.

Let us again write down $u^1(p)$ :

$$u_1(p) : \begin{pmatrix} \sqrt{E-p} \\ 0 \\ \sqrt{E+p} \\ 0 \end{pmatrix}$$

Where $E = +\sqrt{p^2+m^2}$. What is the right way to think about this? Let us draw an analogy to non-relativistic quantum mechanics. We can decompose wavefunctions into a spatial component and a spin part, they nicely factorize. Looking at plane waves solutions of a free particle, we have solutions of the form:

$$e^{i(\boldsymbol{p}\cdot\boldsymbol{x}-Et)}\begin{pmatrix}1\\0\end{pmatrix}$$

[9] This is known as the Feynman slash notation.

Where this is a solution for a spin up free particle. We can make a linear combination of these plane waves to make a general wavefunction:

$$\underbrace{\int d^3p\, f(p)\, e^{i(\boldsymbol{p}\cdot\boldsymbol{x}-Et)}}_{\psi(\boldsymbol{x},t)} \begin{pmatrix}1\\0\end{pmatrix}$$

Suppose we wanted to do the same thing for the plane wave solutions of the Dirac equation:

$$\int d^3p\, f(p)\, u_1(p)\, e^{i(\boldsymbol{p}\cdot\boldsymbol{x}-Et)}$$

However, the components of $u_1(p)$ are not the same, they have different dependences on $p$, and thus we would be left with something of the form:

$$\begin{pmatrix}\phi_1(x,t)\\0\\\phi_2(x,t)\\0\end{pmatrix}$$

The spin/spatial factorization is no longer present in the relativistic theory. In fact, if we take the non-relativistic limit, where $p \to 0$, we see that we recover the factorization.

Let us now discuss the negative energy states. What stops an electron in a finite positive energy state from falling into a negative energy state? According to Dirac, the answer is the Pauli Exclusion Principle. All the negative energy states are normally fully occupied by electrons, which is known as the *Dirac sea*. If this is the case, an electron in a positive energy state, by the Pauli Exclusion Principle, cannot occupy a negative energy state, and thus the negative energy states have no observable consequences. This is a strange concept, but if we think about condensed matter, we often think about the Fermi surface. If the Fermi surface is full, and we insert another electron, the electron cannot interact with the electrons at the Fermi surface, since it is fully occupied. Only if we can introduce enough energy to knock an electron out of the Fermi surface can we see interactions.

Dirac of course did not know about all of this. Instead, his depiction was an infinite band of negative energy states and an infinite band of positive energy states, separated by a band gap of $2mc^2$. The idea was the negative energy band was completely filled, and observable states lived in the positive energy band. The only way to drive interactions between an external electron and the negative band would be to transfer enough energy to knock a negative energy electron into a positive energy state. Only high momentum transfer processes that can cross the “band gap” can interact with the Dirac sea.

Suppose we do knock a negative energy electron out of the sea. In this case, the sea has a net positive charge (since we have a “hole” with a missing electron), and so the sea would appear as a positively charged, positive energy particle. Dirac hated this, but shortly after he developed this idea, the positron was observed, which is exactly the hole state, a positive charge electron.

To summarize, the implications of Dirac’s theory are the aforementioned existence of positrons, and the possibility of pair creation, high energy processes can create electron-positron pairs.

### 3.1.1 Spin in the Dirac Theory

Let us now return to the plane wave solutions and the stated but unproven connection to spin. We expect that the angular momentum of an isolated system is conserved. Let us consider the angular momentum operator $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$ for a single particle, and see if it is conserved. In the Heisenberg picture, we can look at the evolution of the orbital angular momentum in a particular direction:

$$\begin{aligned} i\hbar \frac{dL_z}{dt} &= [L_z, H] \\ &= \left[(xp_y - yp_x), \left(c\boldsymbol{\alpha} \cdot \boldsymbol{p} + mc^2\beta\right)\right] \\ &= [x, p_x]\, c\alpha_x p_y - [y, p_y]\, c\alpha_y p_x \\ &= i\hbar c\left(\alpha_x p_y - \alpha_y p_x\right) \end{aligned}$$

This is not zero! The orbital angular momentum evolves over time, which, if we assume that total angular momentum must be conserved, implies that there is another source of angular momentum. This is the spin angular momentum. The combination of the spin and orbital angular momenta will be conserved, but not the two individually.

Consider the operator $\frac{1}{2}\hbar\Sigma_z$, where $\Sigma_z$ is defined as

$$\Sigma_z = -i\alpha_x\alpha_y$$

We will show that

$$S_z = \frac{1}{2}\hbar\Sigma_z$$

is the spin angular momentum operator in the $z$ direction, and that the sume of the orbital and spin angular momentum will be conserved:

$$\frac{d}{dt}\left(L_z + S_z\right) = 0$$

And via symmetry, we can define the same type of operator for the $x$ and $y$ directions.

Let us now prove this. We can look at the Heisenberg evolution of our defined operator:

$$\begin{aligned} i\hbar \frac{d}{dt}\left(\frac{1}{2}\hbar\Sigma_z\right) &= \frac{1}{2}\hbar\left[\Sigma_z, H\right] \\ &= -\frac{1}{2}i\hbar\left[\alpha_x\alpha_y, c\boldsymbol{\alpha} \cdot \boldsymbol{p} + mc^2\beta\right] \\ &= -\frac{1}{2}i\hbar\left[\left(c\alpha_x\alpha_y\right)\left[\alpha_y, \alpha_x\right] + \left[\alpha_x, \alpha_y\right] c\alpha_y p_y\right] \\ &= i\hbar c\left(\alpha_y p_x - \alpha_x p_y\right) \end{aligned}$$

Where we have used the fact that $\alpha_x\alpha_y\alpha_z = \alpha_z\alpha_x\alpha_y$, and $\alpha_x\alpha_y\beta = \beta\alpha_x\alpha_y$. Note that our result exactly cancels out the result for the time evolution of $L_z$. Thus, this choice of $S_z$, the time derivative of the total angular momentum is zero, and thus this is indeed our spin component. This is historically how the existence of spin-1/2 particles was determined, while we take it for granted that electrons have spin.

More generally, we can define the spin operator:

$$\boldsymbol{S} = \frac{1}{2}\hbar\boldsymbol{\Sigma}$$

Where $\Sigma$ has a cylic property:

$$\begin{aligned}\Sigma_x &= -i\alpha_y\alpha_z \\ \Sigma_y &= -i\alpha_z\alpha_x \\ \Sigma_z &= -i\alpha_x\alpha_y\end{aligned}$$

We can look at the square of the spin operator, noting that $\Sigma_i^2 = 1$:

$$\begin{aligned}\boldsymbol{S}^2 &= \frac{1}{4}\hbar^2\left(\Sigma_x^2 + \Sigma_y^2 + \Sigma_z^2\right) \\ &= \frac{3}{4}\hbar^2\end{aligned}$$

We can explicitly write out $\Sigma_z$:

$$\begin{aligned}\Sigma_z &= i\alpha_x\alpha_y \\ &= \begin{pmatrix}\sigma_3 & 0 \\ 0 & \sigma_3\end{pmatrix}\end{aligned}$$

If we apply our spin operator to what we had labelled the spin up and down solutions:

$$\begin{aligned}S_z w_{\pm\uparrow} &= \frac{1}{2}\hbar w_{\pm\uparrow} \\ S_z w_{\pm\downarrow} &= -\frac{1}{2}\hbar w_{\pm\downarrow}\end{aligned}$$

Which validates our choice of labelling, these are indeed spin up and down.

### 3.1.2 Lorentz Covariance of the Dirac Equation

Let us now discuss the Lorentz covariance of the Dirac equation. Suppose we write down Newton's Second Law:

$$\boldsymbol{F} = m\boldsymbol{a}$$

What does it mean for us to say that $\boldsymbol{a}$ and $\boldsymbol{F}$ are vectors? This is a statement about how they transform under rotations. When we say something is a vector, we say that it transforms like the coordinates do under rotations. We would say that Newton's Second Law is "rotationally covariant". What does this mean? Suppose we have $\boldsymbol{F}$ and $\boldsymbol{a}$ in a particular coordinate system. If we do a coordinate transformation, the equation will still remain true, while the components of $\boldsymbol{F}$ and $\boldsymbol{a}$ are not invariant, both will transform covariantly, the form of the equation will remain invariant.

Now let us do the same for Lorentz transformations of the Dirac equation. We have the Dirac equation:

$$\left(i\gamma^\mu\partial_\mu - m\right)\psi\left(x\right) = 0$$

If someone is in a Lorentz transformed frame, $\psi\left(x\right)$ will not be the same as in your frame. However, the new $\psi\left(x\right)$ in the boosted frame will also satisfy the Dirac equation, the Dirac equation behaves covariantly under rotations and boosts.

Let us now prove this Lorentz covariance. Suppose we have a Lorentz transformation:

$$x^\mu \to x'^\mu = \Lambda^\mu{}_\nu x^\nu$$

We want to show that this leads to $\psi'(x')$ which satisfies:

$$(i\gamma^\mu\partial_\mu - m)\,\psi'\left(x'\right) = 0$$

We can look for a transformation $S$, which depends on $\Lambda$, that transforms between our old and new field:

$$\begin{aligned}\psi'\left(x'\right) &= S(\Lambda)\,\psi(x)\\ &= S(\Lambda)\,\psi\left(\Lambda^{-1}x'\right)\end{aligned}$$

Inverting our original equation, we have that

$$\psi(x) = S^{-1}(\Lambda)\,\psi'\left(x'\right)$$

Similarly, had we done the opposite Lorentz transform $\Lambda^{-1}$, we would have that:

$$\psi(x) = S\left(\Lambda^{-1}\right)\psi'\left(x'\right)$$

These two give us the fact that

$$S^{-1}(\Lambda) = S\left(\Lambda^{-1}\right)$$

Then, the Dirac equation can be written as:

$$(i\gamma^\mu\partial_\mu - m)\,\overbrace{S^{-1}(\Lambda)\,\psi'\left(x'\right)}^{\psi(x)} = 0$$

Now using the chain rule, we can rewrite our $\partial_\mu$:

$$\begin{aligned}\partial_\mu &= \frac{\partial x'^\nu}{\partial x^\mu}\frac{\partial}{\partial x'^\nu}\\ &= \Lambda^\nu{}_\mu\partial'_\nu\end{aligned}$$

Thus the Dirac equation becomes:

$$\left(i\gamma^\mu\Lambda^\nu{}_\mu\partial'_\nu - m\right)S^{-1}(\Lambda)\,\psi'\left(x'\right) = 0$$

Left multiplying by $S(\Lambda)$, we are left with:

$$\left(iS(\Lambda)\,\gamma^\mu S^{-1}(\Lambda)\,\Lambda^\nu{}_\mu\partial'_\nu - m\right)\psi'\left(x'\right) = 0$$

From this, we obtain Lorentz covariance if the following condition on $S(\Lambda)$ is met:

$$S(\Lambda)\,\gamma^\mu S^{-1}(\Lambda)\,\Lambda^\nu{}_\mu = \gamma^\nu$$

How can we find such a $S(\Lambda)$? In this case, it is simpler to look at the infinitesimal case of a transformation. Consider an infinitesimal Lorentz transformation:

$$\Lambda^\nu{}_\mu = \delta^\nu{}_\mu + \Delta w^\nu{}_\mu$$

Which has some associated $S(\Lambda)$, which has some unknown matrix $\sigma_{\mu\nu}$:

$$S = \mathbb{I} - \frac{i}{4}\sigma_{\mu\nu}\Delta w^{\mu\nu}$$

Note that the factor of $\frac{i}{4}$ is placed there with malice aforethought, we will see that there is a convention for $\sigma_{\mu\nu}$, which factors out the $\frac{i}{4}$.

Now let us take our two equations and substitute them into the expression for the requirement on $S$, and drop all terms of order higher than $\Delta w$:

$$\begin{aligned}\left(1-\frac{i}{4}\sigma_{\mu\nu}\Delta w^{\mu\nu}\right)\gamma^\alpha\left(1+\frac{i}{4}\sigma_{\lambda\sigma}\Delta w^{\lambda\sigma}\right)\left(\delta^\beta_\alpha+\Delta w^\beta{}_\alpha\right)&=\gamma^\beta\\ \left(-\frac{i}{4}\sigma_{\mu\nu}\Delta w^{\mu\nu}\right)\gamma^\beta+\gamma^\beta\left(\frac{i}{4}\sigma_{\mu\nu}\Delta w^{\mu\nu}\right)&=-\gamma_\alpha\Delta w^{\beta\alpha}\\ \left(-\frac{i}{4}\sigma_{\mu\nu}\Delta w^{\mu\nu}\right)\gamma^\beta+\gamma^\beta\left(\frac{i}{4}\sigma_{\mu\nu}\Delta w^{\mu\nu}\right)&=\frac{1}{2}\left[-\gamma_\mu\Delta w^{\nu\mu}\delta^\beta_\nu-\gamma_\nu\Delta w^{\mu\nu}\delta^\beta_\mu\right]\end{aligned}$$

Now using the fact that $\Delta w^{\nu\mu}=-\Delta w^{\mu\nu}$, and dividing out by $\Delta w^{\mu\nu}$ on both sides, and rearranging some terms, we are left with:

$$\left[\gamma^\beta,\sigma_{\mu\nu}\right]=-2i\left[\gamma_\mu\delta^\beta_\nu-\gamma_\nu\delta^\beta_\mu\right]$$

Thus we need a $\sigma_{\mu\nu}$ that satisfies this condition, which is independent of the Lorentz transformation that we use.

We claim that the solution is given by:

$$\sigma_{\mu\nu}=\frac{i}{2}\left[\gamma_\mu,\gamma_\nu\right]$$

Let us now verify that this is true. To do this, we need to compute this commutator:

$$\left[\gamma^\beta,\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu\right]$$

Now using a useful property of commutators:

$$[C,AB]=\{A,C\}B-A\{B,C\}$$

Using this, we can compute both parts of the commutator:

$$\begin{aligned}\left[\gamma^\beta,\gamma_\nu\gamma_\mu\right]&=2\delta^\beta_\mu\gamma_\nu-2\gamma_\mu\delta^\beta_\nu\\ \left[\gamma^\beta,\gamma_\nu\gamma_\mu\right]&=2\delta^\beta_\nu\gamma_\mu+2\gamma_\nu\delta^\beta_\mu\end{aligned}$$

From which we have:

$$\left[\gamma^\beta,\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu\right]=4\gamma_\nu\delta^\beta_\mu-4\gamma_\mu\delta^\beta_\nu$$

If we now multiply this by $\frac{i}{2}$, we recover the expected result:

$$\left[\gamma^\beta,\sigma_{\mu\nu}\right]=-2i\left[\gamma_\mu\delta^\beta_\nu-\gamma_\nu\delta^\beta_\mu\right]$$

Thus we have shown that this choice of $\sigma_{\mu\nu}$ works for infinitesimal Lorentz transformations.

Now let us extend this to finite transformations. To do this, we want to build up a finite transformation out of infinitesimal ones. Suppose $\Delta w$ represents the strength of the transformation, and $G^{\nu}{}_{\mu}$ tells us the direction of the transformation:

$$\Delta w^{\nu}{}_{\mu} = \Delta w G^{\nu}{}_{\mu}$$

For example, for a Lorentz transformation along $z$:

$$G^{\nu}{}_{\mu} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

Now let us consider $G^2$:

$$G^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

And let us also note that $G^3 = G$[10]. We can obtain a finite transformation via the limit of a series of the infinitesimal transformations:

$$\begin{aligned} x'^{\nu} &= \lim_{N\to\infty} \left[(\mathbb{I} + \Delta w G)\right]^N x^{\mu} \\ &= \left[e^{N\Delta w G}\right]^{\nu}{}_{\mu} x^{\mu} \\ &= \left[e^{wG}\right]^{\nu}{}_{\mu} x^{\mu} \end{aligned}$$

Where $N\Delta w = w$. Now, rewriting the exponential in terms of hyperbolic sines and cosines:

$$e^{wG} = \cosh(wG) + \sinh(wG)$$

Due to the properties of $G$, we can show that

$$\begin{aligned} \cosh(wG) &= 1 - G^2 + G^2\cosh(w) \\ \sinh(wG) &= G\sinh(w) \end{aligned}$$

To do this, we can series expand the two of them:

$$\cosh(wG) = 1 + \frac{1}{2}w^2G^2 + \frac{1}{4!}w^4G^4 + \dots$$

We can then note that $G^4 = G^2$, since $G^2 = G$, and we are left with:

$$\begin{aligned} \cosh(wG) &= 1 + G^2\left[\frac{1}{2}w^2 + \frac{1}{4!}w^4 + \dots\right] \\ &= 1 + G^2\left[\cosh w - 1\right] \\ &= 1 - G^2 + G^2\cosh(w) \end{aligned}$$

We can use exactly the same logic for the sinh case.

[10] Note the similarity to $SU(3)$ rotations!

Using these two relations, we can rewrite the exponential:

$$e^{wG} = \begin{pmatrix} \cosh(w) & 0 & 0 & -\sinh(w) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh(w) & 0 & 0 & \cosh(w) \end{pmatrix}$$

This is similar to the rotation matrices, except hyperbolic sines and cosines. This is the structure for a finite rotation in coordinate space. Now looking at the field transformation:

$$\begin{aligned} \psi'\left(x'\right) &= S\psi(x) \\ &= \lim_{N\to\infty}\left(1 - \frac{i}{4}\Delta w \sigma_{\mu\nu}G^{\mu\nu}\right)^N \psi(x) \\ &= \exp\left[-\frac{i}{4}(N\Delta w)\sigma_{\mu\nu}G^{\mu\nu}\right]\psi(x) \\ &= \exp\left[-\frac{i}{4}\omega\sigma_{\mu\nu}G^{\mu\nu}\right]\psi(x) \end{aligned}$$

This expression is known as $S(\Lambda)$ :

$$S(\Lambda) = \exp\left[-\frac{i}{4}\omega\sigma_{\mu\nu}G^{\mu\nu}\right]$$

This dictates how spinor fields transform:

$$\psi'\left(x'\right) = S(\Lambda)\psi(x)$$

### 3.1.3 Bilinears of the Dirac Equation

Before we discuss bilinear covariance, let us list some of the important properties of the $\gamma$ matrices, in the basis that we are working in.

We have the defining property:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$$

As well as how we define the dagger:

$$\begin{aligned} \left(\gamma^0\right)^\dagger &= \gamma^0 \\ \left(\gamma^i\right)^\dagger &= -\gamma^i \end{aligned}$$

And we can also write this as:

$$(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0$$

Now let us consider $\overline{\psi} = \psi^\dagger\gamma^0$. We saw how $\psi$ transforms:

$$\psi \to \exp\left[-\frac{i}{4}w\sigma_{\mu\nu}G^{\mu\nu}\right]\psi$$

We can see how $\psi^\dagger$ transforms:

$$\psi^\dagger \to \psi^\dagger \exp\left[\frac{i}{4} w \sigma^\dagger_{\mu\nu} G^{\mu\nu}\right]$$

Using the last property of the gamma matrices we wrote down, we can see that

$$\sigma^\dagger_{\mu\nu} = \gamma^0 \sigma_{\mu\nu} \gamma^0$$

After which we can find how $\overline{\psi}$ transforms:

$$\overline{\psi} \to \overline{\psi} \exp\left[\frac{i}{4} w G^{\mu\nu} \sigma_{\mu\nu}\right]$$

We see that $\psi$ and $\overline{\psi}$ transform in opposite ways, one picks up a negative exponential, and the other picks up a positive exponential. From this, we see that

$$\overline{\psi}\psi$$

is Lorentz invariant.

Let us now define[11] a matrix $\gamma^5$:

$$\begin{aligned} \gamma^5 &= i\gamma^0\gamma^1\gamma^2\gamma^3 \\ &= -\frac{i}{4!}\varepsilon^{\mu\nu\lambda\phi}\gamma_\mu\gamma_\nu\gamma_\lambda\gamma_\phi \end{aligned}$$

We can list some properties of the $\gamma^5$ matrix:

$$\begin{aligned} \left(\gamma^5\right)^\dagger &= \gamma^5 \\ \left(\gamma^5\right)^2 &= \mathbb{I} \\ \{\gamma^5, \gamma^\mu\} &= 0 \end{aligned}$$

In our choice of basis, we have the nice property that $\gamma^5$ is diagonal:

$$\gamma^5 = \begin{pmatrix} -\mathbb{I} & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

Suppose that instead of 3+1D, we were working in 1+1D. In this case, we could just use two of the Pauli matrices as the gamma matrices, in which case $\gamma^5$ would be the third Pauli matrix. If instead we were working in 2+1D, we would have 3 gamma matrices, the Paulis, and there would not be a $\gamma^5$. This has to do with the structure of the Lorentz group, and is why fermions change drastically as we change the dimensionality of our theory.

Let us now list the bilinear covariants of the Dirac equation.

1. $\overline{\psi}\psi$ is a scalar, and there is 1 of these.
2. $\overline{\psi}\gamma^\mu\psi$ is a vector, and there are 4 of these.
3. $\overline{\psi}\sigma^{\mu\nu}\psi$ is a tensor, and there are 6 of these.

[11] Note that the prefactor for $\gamma^5$ is very convention dependent.

4. $\overline{\psi}\gamma^\mu\gamma^5\psi$ is a pseudovector[12], and there are 4 of these.
5. $\overline{\psi}\gamma^5\psi$ is a pseudoscalar, and there is 1 of these.

Thus we have a total of 16 bilinear covariants, combinations of $\overline{\psi}$ and $\psi$ that transform in specific ways under Lorentz transformations. We can also write down a set of basis matrices for all $4 \times 4$ matrices:

$$\{\mathbb{I}, \gamma^\mu, \sigma^{\mu\nu}, \gamma^\mu\gamma^5, \gamma^5\}$$

This is useful, because we can take a look at something very ugly:

$$\overline{\psi}\gamma^\mu\gamma^\nu\gamma^\lambda\gamma^\sigma\gamma^\delta\psi$$

This will reduce to some combination of our irreducible representations (irreps).

# 4 Quantum Field Theory

## 4.1 Second Quantization of the Schrodinger Equation

We shall begin our discussion of quantum field theory via second quantization of the Schrödinger equation.

In a first quantum mechanics course, we take particle motion, quantize, and find wave motion. Suppose instead, we wanted to go the other way, we start with wave motion, quantize, and we will see that we obtain particle motion.

Consider the Lagrangian density:

$$\mathcal{L} = i\hbar\psi^\dagger\dot{\psi} - \frac{\hbar^2}{2m}\boldsymbol{\nabla}\psi^\dagger \cdot \boldsymbol{\nabla}\psi - V\left(\boldsymbol{r}, t\right)\psi^\dagger\psi \tag{10}$$

Where $\psi$ is a complex scalar field. Let treat this the way we would treat a classical Lagrangian density, and find the equation of motion. If we do this, we find equations for both $\psi$ and $\psi^\dagger$ (note that so far, we are treating $\psi$ and $\psi^\dagger$ as separate fields)

$$\begin{aligned} -i\hbar\dot{\psi}^\dagger &= -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi^\dagger + V\left(\boldsymbol{r}, t\right)\psi^\dagger \\ i\hbar\dot{\psi} &= -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V\left(\boldsymbol{r}, t\right)\psi \end{aligned}$$

This looks exactly like the Schrodinger equation (which is exactly why we chose this Lagrangian density to start with). However, $\psi$ is no longer a wavefunction, it is a field.

The canonical momentum conjugate to $\psi$ can be found to be:

$$\begin{aligned} \pi &= \frac{\partial \mathcal{L}}{\partial \dot{\psi}} \\ &= i\hbar\psi^\dagger \end{aligned}$$

[12]pseudo- indicates that it picks up a sign under parity transformations.

The way we interpret this is that $\psi^\dagger$ is not an independent field, $\psi$ is the field, and is the fundamental object. The reason that this is the case is that our Lagrangian density is first order in time derivatives, and only acting on $\psi$, there are no $\dot{\psi}^\dagger$ terms in $\mathcal{L}$ [13].

In the Hamiltonian formalism, $\psi$ and $\pi$ are canonically conjugate variables, and $\psi^\dagger$ is completely determined by $\pi$. Essentially, we started with the assumption that $\psi$ and $\psi^\dagger$ were independent fields, and we have shown that actually, $\psi^\dagger$ is completely dependent on $\psi$.

We can write out the Hamiltonian density:

$$\begin{aligned}\mathcal{H} &= \pi\dot{\psi} - \mathcal{L}\\ &= -\frac{i\hbar}{2m}\boldsymbol{\nabla}\pi\cdot\boldsymbol{\nabla}\psi - \frac{i}{\hbar}V\left(\boldsymbol{r},t\right)\pi\psi\end{aligned}$$

Expressing this in terms of $\psi$ and $\psi^\dagger$:

$$\mathcal{H} = \frac{\hbar^2}{2m}\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\nabla}\psi + V\left(\boldsymbol{r},t\right)\psi^\dagger\psi$$

So far everything has been classical. How do we now quantize this system? To do this, let us recall the elastic rod. We had a collection of masses and springs, and in the discrete case, we wrote down a Lagrangian:

$$L = \frac{1}{2}\sum_i m_i\dot{\eta}_i^2 - \frac{1}{2}k\sum_i\left(\eta_{i+1}-\eta_i\right)^2$$

How would we quantize this classical system? We would introduce a quantization condition between position and conjugate momentum:

$$\left[\eta_i, m\dot{\eta}_i\right] = i\hbar\delta_{ij}$$

And maintain commutation relations between each set of variables:

$$\left[\eta_i,\eta_j\right] = \left[\dot{\eta}_i,\dot{\eta}_j\right] = 0$$

If we did this, we would find that the quantized excitations in the system are phonons. Suppose we now take the continuum limit of this system. To do this, we first rewrite the discrete case using the lattice spacing $a$:

$$\left[\eta_i,\frac{m}{a}\dot{\eta}_j\right] = i\hbar\frac{\delta_{ij}}{a}$$

Taking the continuum limit, we have

$$\left[\eta\left(x\right),\pi\left(x'\right)\right] = i\hbar\delta\left(x-x'\right)$$

Where on the right side, the $1/a$ leads to the Kronecker delta blowing up to infinity, and so we recover a Dirac delta. This is the quantization condition for the classical field in the case of the elastic rod.

The generalization to arbitrary numbers of fields and dimensions is:

$$\left[\eta^\rho\left(x\right),\pi^\rho\left(x'\right)\right] = i\hbar\delta^{D-1}\left(x-x'\right)$$

[13] See the Klein-Gordon theory, in that case, $\pi$ contains derivatives of $\psi$.

$$\left[\eta^{\alpha}(x), \eta^{\beta}(x')\right] = 0$$
$$\left[\pi^{\alpha}(x), \pi^{\beta}(x')\right] = 0$$

Where $D$ is the number of dimensions, In 3+1D, we recover a $\delta^3$. The $\eta^{\rho}(x)$ and $\pi^{\rho}(x)$ are now operators satisfying canonical commutation relations. Let us return to the Schrodinger theory, and apply these commutation relations. In this theory, we have the commutation relations:

$$\left[\hat{\psi}(x), \hat{\pi}(x')\right] = i\hbar\delta^3\left(\boldsymbol{x} - \boldsymbol{x}'\right)$$
$$\left[\hat{\psi}(x), \hat{\psi}(x')\right] = 0$$
$$\left[\hat{\psi}^{\dagger}(x), \hat{\psi}^{\dagger}(x')\right] = 0$$

Inserting the relation between $\hat{\pi}$ and $\hat{\psi}^{\dagger}$, we can rewrite the first commutation relation:

$$\left[\hat{\psi}(x), \hat{\psi}^{\dagger}(x')\right] = \delta^3\left(\boldsymbol{x} - \boldsymbol{x}'\right)$$

These commutation relations are at equal time, $t = t'$. Note that since our operators have time dependence, we are working in the Heisenberg picture. Using the commutation relations, the Heisenberg equation of motion is given by:

$$i\hbar\frac{d\hat{\psi}}{dt} = \left[\hat{\psi}, \hat{H}\right]$$

And we recover the same equation of motion that we found earlier, via the Lagrangian and the Euler-Lagrange equation:

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\hat{\psi} + V(\boldsymbol{r}, t)\,\hat{\psi} = i\hbar\frac{\partial\hat{\psi}}{\partial t}$$

We have spent time discussing what the operators in our theory are, but what about the states? what states do the operators $\hat{\psi}$ and $\hat{\psi}^{\dagger}$ act on? Consider the operator $\hat{N}$:

$$\hat{N} = \int \mathrm{d}^3x\,\hat{\psi}^{\dagger}(x)\,\hat{\psi}(x)$$

It can be verified that

$$\frac{d\hat{N}}{dt} = \left[\hat{N}, \hat{H}\right]$$
$$= 0$$

Thus $\hat{N}$ is a constant of the motion. It also means that $\hat{N}$ and $\hat{H}$ can be simultaneously diagonalized in some basis. Let us now go to a basis in which both $\hat{N}$ and $\hat{H}$ are diagonal.

We can expand the field operators in terms of eigenfunctions of the Hamiltonian:

$$\hat{\psi}(\boldsymbol{x}, t) = \sum_k \hat{\hat{a}}_k(t)\,u_k(\boldsymbol{x})$$
$$\hat{\psi}^{\dagger}(\boldsymbol{x}, t) = \sum_k \hat{\hat{a}}_k(t)\,u_k^*(\boldsymbol{x})$$

Where $u_k\left(\boldsymbol{x}\right)$ satisfies the condition:

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 u_k\left(\boldsymbol{x}\right)+V\left(\boldsymbol{x}\right)u_k\left(\boldsymbol{x}\right)=E_k u_k\left(\boldsymbol{x}\right)$$

Where we have restricted our system to have a time-independent potential $V\left(\boldsymbol{x}\right)$. The $u_k\left(\boldsymbol{x}\right)$ are eigenfunctions of a Hermitian operator, so they are orthogonal, and they form a complete set. We could have expanded our field operators in any set of orthogonal functions (sines/cosines, etc.), but we chose the $u_k\left(\boldsymbol{x}\right)$ functions because we want to diagonalize the Hamiltonian.

Recall that the Hamiltonian density was given by

$$\mathcal{H}=\frac{\hbar^2}{2m}\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\nabla}\psi+V\left(\boldsymbol{x}\right)\psi^\dagger\psi$$

The Hamiltonian is the integration of the density:

$$\begin{aligned}H&=\int \mathrm{d}^3x\,\mathcal{H}\\&=\int \mathrm{d}^3x\,\hat{\psi}^\dagger\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\hat{\psi}+V\left(\boldsymbol{x}\right)\hat{\psi}\right]\end{aligned}$$

Where we have integrated by parts to pull out the $\hat{\psi}^\dagger$. If we now insert our expanded field operators into this, and use the fact that $u_k\left(\boldsymbol{x}\right)$ are eigenfunctions of the Hamiltonian, we will be able to reduce the whole expression.

Suppose we take the equation of motion, and substitute in our expanded operators:

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\hat{\psi}+V\left(\boldsymbol{x}\right)\hat{\psi}=i\hbar\frac{\partial\hat{\psi}}{\partial t}$$

Before doing this, we note that

$$i\hbar\frac{d\hat{\hat{a}}_k}{dt}=E_k\hat{\hat{a}}_k$$

From which we find that

$$\hat{\hat{a}}_k\left(t\right)=\hat{a}_k e^{-iE_kt/\hbar}$$

From this, we have that our expanded operators take the form:

$$\begin{aligned}\hat{\psi}\left(\boldsymbol{x},t\right)&=\sum_k\hat{a}_k u_k\left(\boldsymbol{x}\right)e^{-iE_kt/\hbar}\\\hat{\psi}^\dagger\left(\boldsymbol{x},t\right)&=\sum_k\hat{a}_k^\dagger u_k^*\left(\boldsymbol{x}\right)e^{iE_kt/\hbar}\end{aligned}$$

We see that we can extract the time dependence from our Fourier coefficient operators. Now we can invert this equations (just as one does to find Fourier coefficients) to find $\hat{a}_k$ and $\hat{a}_k^\dagger$, via the fact that the $u_k$ functions provide an orthogonal basis of functions. Let us assume that we have a normalization condition:

$$\int \mathrm{d}^3x\,u_k^*\left(\boldsymbol{x}\right)u_l\left(\boldsymbol{x}\right)=\delta_{kl}$$

Inverting our expansions, we find that

$$\hat{a}_k = \int \mathrm{d}^3\boldsymbol{x}\, \hat{\psi}\left(\boldsymbol{x}, t\right) u_k^*\left(\boldsymbol{x}\right) e^{iE_k t/\hbar}$$
$$\hat{a}_k^\dagger = \int \mathrm{d}^3\boldsymbol{x}\, \hat{\psi}^\dagger\left(\boldsymbol{x}, t\right) u_k\left(\boldsymbol{x}\right) e^{-iE_k t/\hbar}$$

Since we know the commutation relations between $\hat{\psi}$ and $\hat{\psi}^\dagger$, we can use these to find the commutation relations between $\hat{a}_k$ and $\hat{a}_k^\dagger$:

$$\left[\hat{a}_k, \hat{a}_l\right] = 0$$
$$\left[\hat{a}_k^\dagger, \hat{a}_l^\dagger\right] = 0$$

These follow from the fact that $\hat{a}$ and $\hat{a}^\dagger$ only depend on $\hat{\psi}$ and $\hat{\psi}^\dagger$ respectively, and those commute with each other. The final commutator requires a bit more work:

$$\begin{aligned}
\left[\hat{a}_k, \hat{a}_l^\dagger\right] &= \int \mathrm{d}^3x \int \mathrm{d}^3x'\, e^{i(E_k - E_l)t/\hbar} u_k^*\left(\boldsymbol{x}\right) u_l\left(\boldsymbol{x}'\right) \overbrace{\left[\hat{\psi}\left(\boldsymbol{x}, t\right), \hat{\psi}^\dagger\left(\boldsymbol{x}', t\right)\right]}^{\delta^3(\boldsymbol{x}-\boldsymbol{x}')} \\
&= e^{i(E_k - E_l)t/\hbar} \int \mathrm{d}^3x\, u_k^*\left(\boldsymbol{x}\right) u_l\left(\boldsymbol{x}\right) \\
&= \delta_{kl}
\end{aligned}$$

Now let us return to the Hamiltonian and number operator. Let us rewrite these in terms of $\hat{a}_k$ and $\hat{a}_k^\dagger$:

$$\begin{aligned}
\hat{N} &= \int \mathrm{d}^3x\, \hat{\psi}^\dagger\left(\boldsymbol{x}, t\right) \\
&= \int \mathrm{d}^3x \sum_l \hat{a}_l^\dagger u_l^*\left(\boldsymbol{x}\right) e^{iE_l t/\hbar} \sum_k \hat{a}_k u_k\left(\boldsymbol{x}\right) e^{-iE_k t/\hbar} \\
&= \sum_{l,k} \hat{a}_l^\dagger \hat{a}_k e^{i(E_l - E_k)t/\hbar} \int \mathrm{d}^3x\, u_k\left(\boldsymbol{x}\right) u_l^*\left(\boldsymbol{x}\right) \\
&= \sum_k \hat{a}_k^\dagger \hat{a}_k
\end{aligned}$$

Where we note that the only terms that depend on $\boldsymbol{x}$ in the integral are the functions $u_l^*\left(\boldsymbol{x}\right)$ and $u_k\left(\boldsymbol{x}\right)$, so we can use the orthogonality relation to remove the integral and get a Kronecker delta, and then use that to collapse the two sums into one. It is also useful to define an operator $\hat{N}_k$:

$$\hat{N}_k = \hat{a}_k^\dagger \hat{a}_k$$

From which we have

$$\hat{N} = \sum_k \hat{N}_k$$

Let us do the same process for the Hamiltonian:

$$\hat{H} = \int \mathrm{d}^3\boldsymbol{x}\, \frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 \hat{\psi}^\dagger \cdot \boldsymbol{\nabla}\hat{\psi} + V\left(\boldsymbol{x}\right) \hat{\psi}^\dagger \hat{\psi}$$

$$
\begin{aligned}
&= \sum_{k,l} \hat{a}_k^\dagger \hat{a}_l e^{i(E_k - E_l)t/\hbar} \int \mathrm{d}^3\boldsymbol{x} \left( \frac{\hbar^2}{2m} \boldsymbol{\nabla} u_k^* \cdot \boldsymbol{\nabla} u_l + u_k^* V\left(\boldsymbol{x}\right) u_l \right) \\
&= \sum_{k,l} \hat{a}_k^\dagger \hat{a}_l e^{i(E_k - E_l)t/\hbar} \int \mathrm{d}^3\boldsymbol{x}\, u_k^* \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 u_l + V\left(\boldsymbol{x}\right) u_l \right) \\
&= \sum_{k,l} \hat{a}_k^\dagger \hat{a}_l e^{i(E_k - E_l)t/\hbar} \int \mathrm{d}^3\boldsymbol{x}\, u_k^* \left( E_l u_l \right) \\
&= \sum_{k,l} \hat{a}_k^\dagger \hat{a}_l e^{i(E_k - E_l)t/\hbar} E_l \delta_{kl} \\
&= \sum_{k} E_k \hat{a}_k^\dagger \hat{a}_k \\
&= \sum_{k} E_k \hat{N}_k
\end{aligned}
$$

Where we integrate by parts, and drop the boundary term, under the assumption that the eigenfunctions vanish at infinity. We then use the fact that $u_l$ is by definition an eigenfunction of the Schrodinger equation, and then we use the orthogonality condition to get a Kronecker delta and collapse the integral and two sums into a single sum.

Now how do we find the eigenvalues of the Hamiltonian? First, let us note that $\left[\hat{N}_i, \hat{N}_j\right] = 0$. Because of this, we can diagonalize them simultaneously. Thus, finding the eigenvalues of the Hamiltonian boils down to finding the eigenvalues of $\hat{N}_k$. Now recall the harmonic oscillator from quantum mechanics. We can write the oscillator Hamiltonian as:

$$
\hat{H}_{\text{osc}} = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right)
$$

The raising and lowering operators satisfied the same commutation relations that we have for our Schrodinger field, and in the case of the oscillator, eigenvalues of $a^\dagger a$ were integers. Thus, if we can reproduce this argument, we can get the eigenvalues of our Schrodinger field Hamiltonian.

Consider the commutator:

$$
\begin{aligned}
\left[\hat{N}_i, \hat{a}_i\right] &= \left[\hat{a}_i \hat{a}_i, \hat{a}_i\right] \\
&= \left[\hat{a}_i^\dagger, \hat{a}_i\right] \hat{a}_i \\
&= -\hat{a}_i
\end{aligned}
$$

Similarly, we can compute the commutator with $\hat{a}_i^\dagger$ :

$$
\left[\hat{N}_i, \hat{a}_i^\dagger\right] = \hat{a}_i^\dagger
$$

Now let $\left|n_i\right\rangle$ be an eigenstate of $\hat{N}_i$, with eigenvalue $n_i$:

$$
\hat{N}_i \left|n_i\right\rangle = n_i \left|n_i\right\rangle
$$

Now, consider applying $\hat{N}_i$ to the eigenstate that has $\hat{a}_i$ applied to it:

$$
\begin{aligned}
\hat{N}_i \left( \hat{a}_i \left|n_i\right\rangle \right) &= \left[\hat{N}_i, \hat{a}_i\right] \left|n_i\right\rangle + \hat{a}_i \hat{N}_i \left|n_i\right\rangle \\
&= -\hat{a}_i \left|n_i\right\rangle + n_i \hat{a}_i \left|n_i\right\rangle
\end{aligned}
$$

$$= (n_i - 1)\,\hat{a}_i\,|n_i\rangle$$

From this, we see that $\hat{a}_i\,|n_i\rangle$ is an eigenstate of $\hat{N}_i$, with eigenvalue $n_i - 1$, and therefore this is the state $|n_i - 1\rangle$. From here, we can keep applying $\hat{a}_i$, and continuing lowering the eigenvalue and the eigenstate label. To prove that $n_i$ must be a positive integer, we note that $\langle\hat{N}_i\rangle_\psi$ must be positive, $\hat{N}_i$ is a positive definite operator[14]:

$$\begin{aligned}\langle\psi|\hat{N}_i|\psi\rangle &= \langle\psi|\,\hat{a}_i^\dagger\,(\hat{a}_i\,|\psi\rangle) \\ &= \langle\phi|\phi\rangle \geq 0\end{aligned}$$

Thus, by repeatedly applying $\hat{a}_i$ to $|n_i\rangle$, it appears that one can continue decreasing the eigenvalue infinitely. However, since $\hat{N}_i$ is positive definite, all of its eigenvalues are positive. Therefore, the only way that we resolve this is if we have a state labelled $|0\rangle_i$, with eigenvalue 0:

$$\hat{a}_i\,|0_i\rangle = 0\,|0_i\rangle$$

Then, applying $\hat{N}_i$ will also give us zero:

$$\hat{N}_i\,|0_i\rangle = 0\,|0_i\rangle$$

So $|0_i\rangle$ is an eigenvector of $\hat{N}_i$ with eigenvalue 0. Due to the unit spacing of the eigenvalues, the eigenvalues of $\hat{N}_i$ are $0, 1, 2, \ldots$, and the corresponding eigenvectors are $|0_i\rangle, |1_i\rangle, |2_i\rangle, \ldots$. Since all the $\hat{N}_i$s can be independently diagonalized, an eigenstate of all of the $\hat{N}_i$ operators as:

$$|n_1, n_2, \ldots, n_i, \ldots\rangle$$

Given this state, we can see what the action of a single one of the $\hat{N}_i$ operators will be:

$$\hat{N}_i\,|n_1, n_2, \ldots, n_i, \ldots\rangle = n_i\,|n_1, n_2, \ldots, n_i, \ldots\rangle$$

From this, we have that the eigenvalues of the full $\hat{N}$ operator are given by:

$$\hat{N}\,|n_1, n_2, \ldots, n_i, \ldots\rangle = \sum_i n_i\,|n_1, n_2, \ldots, n_i, \ldots\rangle$$

Which immediately gives us the eigenvalues of the Hamiltonian:

$$\hat{H}\,|n_1, n_2, \ldots, n_i, \ldots\rangle = \left(\sum_i n_i E_i\right)|n_1, n_2, \ldots, n_i, \ldots\rangle$$

How do we interpret this? We interpret $n_1$ as the number of particles in energy level 1, and generalizing, $n_i$ is the number of particles in the $i$th energy level. From this, the eigenvalue of $\hat{N}$ gives us the total number of particles in our system.

We solved this for an arbitrary potential $V(\boldsymbol{x})$. All of the particles in the system are interacting with the potential, but they are not interacting with each other. The problem that we have solved is therefore analogous to $\sum_i n_i$ noninteracting particles distributed among the energy eigenstates generated by the potential $V(\boldsymbol{x})$. We see that even though we started with a single particle Schrodinger equation, the solution gave us the dynamics of an *arbitrary* number of particles in the system.

[14] Not all Hermitian matrices are positive definite!

Now we return to our $\hat{a}_i$ operator, and we see that it can decrement the number of particles in the $i$th energy level:

$$\hat{a}_i \left|n_1, n_2, \ldots n_i, \ldots\right\rangle \propto \left|n_1, n_2, \ldots, n_i - 1, \ldots\right\rangle$$

Similarly, $\hat{a}_i^\dagger$ increments the number of particles in the $i$th energy level:

$$\hat{a}_i^\dagger \left|n_1, n_2, \ldots, n_i, \ldots\right\rangle \propto \left|n_1, n_2, \ldots, n_i + 1, \ldots\right\rangle$$

For this reason, $\hat{a}_i$ is known as the annihilation operator, and $\hat{a}_i^\dagger$ is known as the creation operator.

The state with no particles, $\left|0, 0, 0 \ldots\right\rangle$ is known as the vacuum.

Now suppose we want to take what we have just found, and return to the usual way we think about quantum mechanics. Let us consider the action of the operators $\hat{\psi}(x)$ and $\hat{\psi}^\dagger(x)$ on the vacuum. Let us suppose this state is denoted $\left|\boldsymbol{x}, t\right\rangle$ :

$$\hat{\psi}^\dagger(\boldsymbol{x}, t)\left|0\right\rangle = \left|\boldsymbol{x}, t\right\rangle$$

Note that the action of $\psi(\boldsymbol{x}, t)$ on the vacuum must be zero, since it contains just a $\hat{a}$. Let us now consider the time derivative of this state:

$$i\hbar\frac{\partial}{\partial t}\left|\boldsymbol{x}, t\right\rangle = i\hbar\frac{\partial}{\partial t}\hat{\psi}^\dagger(\boldsymbol{x}, t)\left|0\right\rangle$$

Now using the Heisenberg picture evolution of the operator $\hat{\psi}^\dagger$, where $\left|0\right\rangle$ is constant in time:

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{\psi}^\dagger(\boldsymbol{x}, t)\left|0\right\rangle &= \left[\hat{\psi}^\dagger, \hat{H}\right]\left|0\right\rangle \\
&= -\hat{H}\hat{\psi}^\dagger(\boldsymbol{x}, t)\left|0\right\rangle \\
&= -\hat{H}\left|\boldsymbol{x}, t\right\rangle
\end{aligned}$$

We see that this is very reminiscent of the Schrodinger equation, but we have the wrong sign. Now let us consider the inner product of two of these states:

$$\begin{aligned}
\left\langle\boldsymbol{x}', t \middle| \boldsymbol{x}, t\right\rangle &= \left\langle 0\right|\hat{\psi}\left(\boldsymbol{x}', t\right)\hat{\psi}^\dagger(\boldsymbol{x}, t)\left|0\right\rangle \\
&= \left\langle 0\right|\left[\hat{\psi}\left(\boldsymbol{x}', t\right), \hat{\psi}^\dagger(\boldsymbol{x}, t)\right]\left|0\right\rangle \\
&= \delta^3\left(\boldsymbol{x} - \boldsymbol{x}'\right)
\end{aligned}$$

Where we note that we can replace the product of our two operators with the commutator since the second term in the commutator vanishes, $\hat{\psi}$ acting on the vacuum is zero. The object that satisfies the Schrodinger equation with the wrong sign and has this normalization condition is the position basis vector in the Heisenberg picture. This suggests that $\left|\boldsymbol{x}, t\right\rangle$ are basis vectors for single particle states in the Heisenberg picture. Given a time-independent single particle state vector $\left|\psi\right\rangle$, the position space wavefunction is given by

$$\left\langle\boldsymbol{x}, t \middle| \psi\right\rangle = \psi(\boldsymbol{x}, t)$$

Let us confirm this by constructing the wavefunction of the statevector

$$\left|0, 0, \ldots 1_i, \ldots\right\rangle$$

which is a single particle in the $i$th energy eigenstate. We relabel this state as $|i\rangle$:

$$|i\rangle = \hat{a}_i^\dagger |0\rangle$$

The wavefunction of $|i\rangle$ is:

$$\begin{aligned}
\langle \boldsymbol{x}, t | i \rangle &= \langle 0 | \hat{\psi}(\boldsymbol{x}, t) \, \hat{a}_i^\dagger | 0 \rangle \\
&= \left\langle 0 \middle| \hat{\psi}(\boldsymbol{x}, t) \int \mathrm{d}^3\boldsymbol{x} \, \hat{\psi}^\dagger(\boldsymbol{x}', t) \, u_i(\boldsymbol{x}) \, e^{-iE_i t/\hbar} \middle| 0 \right\rangle \\
&= e^{-iE_i t/\hbar} \int \mathrm{d}^3\boldsymbol{x} \, u_i(\boldsymbol{x}) \underbrace{\langle 0 | \left[\hat{\psi}(\boldsymbol{x}, t), \hat{\psi}^\dagger(\boldsymbol{x}', t)\right] | 0 \rangle}_{\delta^3(\boldsymbol{x}-\boldsymbol{x}')} \\
&= u_i(\boldsymbol{x}) \, e^{-iE_i t/\hbar}
\end{aligned}$$

Which is exactly the time-dependent wavefunction for a particle in the $i$th energy eigenstate.

Thus we have shown that we can take a state and construct its wavefunction. Suppose instead we had a wavefunction, and we wanted to construct the state with that particular wavefunction at some time $t = t'$. Consider the operator $\hat{\psi}_s^\dagger(\boldsymbol{x}, t, t')$, defined as:

$$\hat{\psi}_s^\dagger(\boldsymbol{x}, t, t') = e^{-i\hat{H}(t-t')/\hbar} \hat{\psi}^\dagger(\boldsymbol{x}, t) \, e^{i\hat{H}(t-t')/\hbar}$$

The $s$ subscript denotes Schrodinger, as we can see that this object does not evolve in time. Thus, when we apply this to the vacuum, we create states that do not evolve in time, which is what we want when working in the Heisenberg picture. Let us show that this is time independent:

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{\psi}_s^\dagger(\boldsymbol{x}, t, t') &= e^{-i\hat{H}(t-t')/\hbar} \left( \hat{H}\hat{\psi}^\dagger + i\hbar\frac{\partial \hat{\psi}^\dagger}{\partial t} - \hat{\psi}^\dagger \hat{H} \right) E^{i\hat{H}(t-t')/\hbar} \\
&= e^{-i\hat{H}(t-t')/\hbar} \left( \hat{H}\hat{\psi}^\dagger + \left[\hat{\psi}^\dagger, \hat{H}\right] - \hat{\psi}^\dagger \hat{H} \right) E^{i\hat{H}(t-t')/\hbar} \\
&= 0
\end{aligned}$$

Where we have applied the Heisenberg equation of motion for $\hat{\psi}^\dagger$. Thus we see that $\hat{\psi}_s^\dagger$ is actually independent of $t$:

$$\hat{\psi}_s^\dagger(\boldsymbol{x}, t, t') = \hat{\psi}_s^\dagger(\boldsymbol{x}, t')$$

Now consider the statevector given by the action of this operator on the vacuum

$$\hat{\psi}_s^\dagger(\boldsymbol{x}, t') |0\rangle$$

We claim that this represents a single particle state localized at $\boldsymbol{x}$, at time $t = t'$. To see this, we can project it against the basis vectors:

$$\langle \boldsymbol{x}', t | \hat{\psi}_s^\dagger(\boldsymbol{x}, t') |0\rangle = \left\langle 0 \middle| \hat{\psi}(\boldsymbol{x}', t) \, e^{-i\hat{H}(t-t')/\hbar} \hat{\psi}^\dagger(\boldsymbol{x}, t) \, e^{i\hat{H}(t-t')/\hbar} \middle| 0 \right\rangle$$

At time $t = t'$, this is exactly a delta function, $\delta^3(\boldsymbol{x} - \boldsymbol{x}')$. What if we look at the time derivative of this object?

$$i\hbar\frac{\partial}{\partial t} \langle \boldsymbol{x}', t | \hat{\psi}_s^\dagger(\boldsymbol{x}, t') |0\rangle = i\hbar\frac{\partial}{\partial t} \langle 0 | \hat{\psi}(\boldsymbol{x}', t) \, \hat{\psi}_s(\boldsymbol{x}, t') |0\rangle$$

$$
\begin{aligned}
&= \left\langle 0 \left| i\hbar \frac{\partial}{\partial t} \hat{\psi}\left(\boldsymbol{x}', t\right) \hat{\psi}_s^\dagger\left(\boldsymbol{x}, t'\right) \right| 0 \right\rangle \\
&= \left\langle 0 \left| \left[ -\frac{\hbar^2}{2m} \boldsymbol{\nabla}'^2 \hat{\psi} + V\left(\boldsymbol{x}'\right) \hat{\psi} \right] \hat{\psi}_s^\dagger\left(\boldsymbol{x}, t'\right) \right| 0 \right\rangle \\
&= \left[ -\frac{\hbar^2}{2m} \boldsymbol{\nabla}'^2 + V\left(\boldsymbol{x}'\right) \right] \langle 0 | \hat{\psi}\left(\boldsymbol{x}', t\right) \hat{\psi}_s^\dagger\left(\boldsymbol{x}, t'\right) | 0 \rangle \\
&= \left[ -\frac{\hbar^2}{2m} \boldsymbol{\nabla}'^2 + V\left(\boldsymbol{x}'\right) \right] \langle \boldsymbol{x}', t | \hat{\psi}_s^\dagger\left(\boldsymbol{x}, t'\right) | 0 \rangle
\end{aligned}
$$

We see that the state evolves in time according the Schrodinger equation, which is exactly what we would expect. Now that we have proven that it has the correct time evolution, as well as the correct localization, we have shown that this state is indeed a single particle state localized at $\boldsymbol{x}$, at time $t = t'$.

Suppose we now want an arbitrary one-particle state $|f\rangle$ with wavefunction $f(\boldsymbol{x})$ at time $t = t'$. We can construct this via the delta function state:

$$
|f\rangle = \int \mathrm{d}^3\boldsymbol{x}\, f(\boldsymbol{x})\, \hat{\psi}_s^\dagger\left(\boldsymbol{x}, t'\right) |0\rangle
$$

It is straightforward to verify that the wavefunction of $|f\rangle$, $\langle \boldsymbol{x}, t | f \rangle$ is indeed $f(\boldsymbol{x})$ at time $t = t'$ and satisfies the Schrodinger wave equation, by following the exact same steps we used in the delta function case.

Now suppose we looked at $\langle \boldsymbol{x}, t | f \rangle$:

$$
\begin{aligned}
\langle \boldsymbol{x}, t | f \rangle &= \langle 0 | \hat{\psi}(\boldsymbol{x}, t) | f \rangle \\
&= \langle 0 | \hat{\psi}(\boldsymbol{x}, t) \left( \int \mathrm{d}^3\boldsymbol{x}\ |\boldsymbol{x}', t'\rangle \langle \boldsymbol{x}', t'| \right) |f\rangle \\
&= \int \mathrm{d}^3\boldsymbol{x}\ \langle 0 | \hat{\psi}(\boldsymbol{x}, t)\, \hat{\psi}^\dagger\left(\boldsymbol{x}', t'\right) | 0 \rangle \langle \boldsymbol{x}', t' | f \rangle
\end{aligned}
$$

We see that the second term is the wavefunction at time $t'$, and the other inner product is the Greens function, known as the propagator:

$$
G\left(\boldsymbol{x}, \boldsymbol{x}'; t, t'\right) = \langle 0 | \hat{\psi}(\boldsymbol{x}, t)\, \hat{\psi}^\dagger\left(\boldsymbol{x}', t'\right) | 0 \rangle \tag{11}
$$

The propagator encompasses the time dependence of the state. Suppose we rewrite the propagator in the energy eigenbasis, using $\hat{a}_k$ and $\hat{a}_k^\dagger$. If we did this, we would recover the familiar form of the non-relativistic propagator:

$$
G\left(\boldsymbol{x}, \boldsymbol{x}'; t, t'\right) = \sum_k u_k(\boldsymbol{x})\, u_k^*\left(\boldsymbol{x}'\right) e^{-iE_k(t-t')/\hbar}
$$

In a certain sense we have not done anything new here, this is a mathematically equivalent way of doing quantum mechanics, everything we have done could be done by working in the traditional quantum mechanics formalism.

### 4.1.1 Multi-Particle States

Now let us turn our attention to multi-particle states, starting with 2 particle states. For any 2 particle state $|f\rangle$, the wavefunction can be found by using two $\hat{\psi}$ operators, rather than just one:

$$f\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t\right)=\langle 0| \hat{\psi}\left(\boldsymbol{x}_1, t\right) \hat{\psi}\left(\boldsymbol{x}_2, t\right)|f\rangle$$

This satisfies the Schrodinger equation:

$$\begin{aligned} i \hbar \frac{\partial}{\partial t}\langle 0| \hat{\psi}\left(\boldsymbol{x}_1, t\right) \hat{\psi}\left(\boldsymbol{x}_2, t\right)|f\rangle &=\langle 0| i \hbar \frac{\partial}{\partial t} \hat{\psi}\left(\boldsymbol{x}_1, t\right) \hat{\psi}\left(\boldsymbol{x}_2, t\right)|f\rangle+\langle 0| \hat{\psi}\left(\boldsymbol{x}_1, t\right) i \hbar \frac{\partial}{\partial t} \hat{\psi}\left(\boldsymbol{x}_2, t\right)|f\rangle \\ &=\left[-\frac{\hbar^2}{2 m}\left(\boldsymbol{\nabla}_1^2+\boldsymbol{\nabla}_2^2\right)+V\left(\boldsymbol{x}_1\right)+V\left(\boldsymbol{x}_2\right)\right]\langle 0| \hat{\psi}\left(\boldsymbol{x}_1, t\right) \hat{\psi}\left(\boldsymbol{x}_2, t\right)|f\rangle \end{aligned}$$

Where we have inserted the equations of motion for both single-particle wavefunctions. We see that this object satisfies the two particle Schrodinger equation, as we would expect. Also note that the $\hat{\psi}$ operators commute, and therefore the object is symmetric under interchange of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, and therefore this can only describe bosonic particles. This constraint was introduced by the canonical commutation relations that we imposed on the fields.

Thus we have shown that given a statevector, we can extract its wavefunction. To do the converse, where we want to construct a state with wavefunction $f\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)$ at time $t'$, we can generalize the single particle case, by introducing another $\hat{\psi}_s^{\dagger}$, and integrating over another set of coordinates:

$$\int \mathrm{d}^3 \boldsymbol{x}_1 \int \mathrm{d}^3 \boldsymbol{x}_2\, f\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right) \hat{\psi}_s^{\dagger}\left(\boldsymbol{x}_1, t'\right) \hat{\psi}_s^{\dagger}\left(\boldsymbol{x}_2, t'\right)|0\rangle$$

The generalization to higher particle count states is straightforward. Notice that the $\hat{\psi}_s^{\dagger}$ operators commute, so again this will be symmetric in $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, regardless of whether $f\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)$ is symmetric under interchange. Suppose we chose an $f$ that does not have symmetry. If we then wrote this object down and exchanged $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, and then used the fact that the operators commute and we can switch the order of integration:

$$\int \mathrm{d}^3 \boldsymbol{x}_2 \int \mathrm{d}^3 \boldsymbol{x}_1\, f\left(\boldsymbol{x}_2, \boldsymbol{x}_1\right) \hat{\psi}_s^{\dagger}\left(\boldsymbol{x}_2, t'\right) \hat{\psi}_s^{\dagger}\left(\boldsymbol{x}_1, t'\right)|0\rangle=\int \mathrm{d}^3 \boldsymbol{x}_1 \int \mathrm{d}^3 \boldsymbol{x}_2\, f\left(\boldsymbol{x}_2 . \boldsymbol{x}_1\right) \hat{\psi}_s^{\dagger}\left(\boldsymbol{x}_1, t'\right) \hat{\psi}_s^{\dagger}\left(\boldsymbol{x}_2, t'\right)|0\rangle$$

So in fact the only part of $f$ that survives is the symmetrized portion:

$$\frac{1}{2}\left[f\left(\boldsymbol{x}_1, \boldsymbol{x}_2\right)+f\left(\boldsymbol{x}_2, \boldsymbol{x}_1\right)\right]$$

The construction of the state automatically takes into account the statistics of the bosons, since we imposed the canonical commutation relations. How can we recover Fermi-Dirac statistics? Recall the two particle wavefunction:

$$f\left(\boldsymbol{x}_1, \boldsymbol{x}_2, t\right)=\langle 0| \hat{\psi}\left(\boldsymbol{x}_1, t\right) \hat{\psi}\left(\boldsymbol{x}_2, t\right)|f\rangle$$

Suppose we required that the $\hat{\psi}$ operators *anti*commute, rather than commute. In that case, we would recover the fermionic antisymmetry of the wavefunction, exchanging $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ would introduce a minus sign. The issue is whether or not this anticommutation requirement is consistent with all of the rest of the theory that we have worked through, under the assumption that the operators commute. Instead of imposing the canonical commutation relations, let us impose the canonical *anticommutation* relations (equal time):

$$\begin{aligned}
\{\hat{\psi}(\boldsymbol{x},t),\hat{\psi}(\boldsymbol{x}',t)\} &= 0\\
\{\hat{\pi}(\boldsymbol{x},t),\hat{\pi}(\boldsymbol{x}',t)\} &= 0\\
\{\hat{\psi}(\boldsymbol{x},t),\hat{\pi}(\boldsymbol{x}',t)\} &= i\hbar\delta^3(\boldsymbol{x}-\boldsymbol{x}')
\end{aligned} \tag{12}$$

Let us start from the same Lagrangian density (10):

$$\mathcal{L} = i\hbar\psi^\dagger\frac{\partial\psi}{\partial t} - \frac{\hbar^2}{2m}\boldsymbol{\nabla}\psi^\dagger\cdot\boldsymbol{\nabla}\psi - V(\boldsymbol{x})\,\psi^\dagger\psi$$

Where $\psi$ is a complex scalar field. Recall that the equation of motion is:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V\psi$$

And we have a conjugate momentum $\pi = \frac{\partial\mathcal{L}}{\partial\dot{\psi}} = i\hbar\psi^\dagger$, and this gives us the Hamiltonian density:

$$\begin{aligned}
\mathcal{H} &= \pi\dot{\psi} - \mathcal{L}\\
&= \frac{\hbar^2}{2m}\boldsymbol{\nabla}\psi\dagger\cdot\boldsymbol{\nabla}\psi + V(\boldsymbol{x})\,\psi^\dagger\psi
\end{aligned}$$

So far, everything has been classical. Now let us impose our canonical anticommutation relations (12), and let us make note of the fact that the constant in front the delta function vanishes:

$$\{\psi(\boldsymbol{x}),\psi^\dagger(\boldsymbol{x}')\} = \delta^3(\boldsymbol{x}-\boldsymbol{x}')$$

We will skip many of the derivations that are analogous to the bosonic case[15]. If we combine our imposed anticommutation relations with the Heisenberg equation of motion:

$$i\hbar\frac{\partial\hat{\psi}}{\partial t} = \left[\hat{\psi},\hat{H}\right]$$

we obtain the same equation of motion that we obtained from the Lagrangian. This is a good start!

[15] Exercises left to the homework-doer.