Second quantization: where quantization and particles come from?

### 7.1. Lagrangian mechanics and canonical quantization

**Q:** How do we quantize a general system?

#### 7.1.1. Lagrangian

Lagrangian mechanics is a reformulation of classical mechanics.

\[ L = T - V \]  

(7.1)

Here, the quantity \( L \) is called the Lagrangian, where \( T \) is the kinetic energy and \( V \) is the potential energy.

For example, for a pendulum as shown in the figure, the kinetic energy is

\[ T = \frac{1}{2} m r^2 \left( \frac{d\theta}{dt} \right)^2 = \frac{1}{2} m r \dot{\theta}^2 \]  

(7.2)

where \( \dot{\theta} \) represents time derivative of \( \theta \)

\[ V = -m g r \cos \theta \]  

(7.3)

And thus

\[ L(\dot{\theta}, \theta) = \frac{1}{2} m r^2 \dot{\theta}^2 + m g r \cos \theta \]  

(7.4)

Here, the Lagrangian depends on \( \theta \) and the time derivative of \( \theta \). In Lagrangian mechanics, \( \theta \) is called a coordinate. In this example, we have only one single coordinate, but in general, a more complicated system can have multiple coordinates. And in general, \( L \) depends on the coordinates and the time derivatives of these coordinates, e.g.

\[ L(q_1, \dot{q}_1; q_2, \dot{q}_2; \ldots; q_n, \dot{q}_n) \]  

(7.5)

where \( q_i \) are coordinates.

#### 7.1.2. Equation(s) of motion

The equation of motion in Lagrangian mechanics:

\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0 \]  

(7.6)

For the pendulum example discussed above,
\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = \frac{\partial L}{\partial \theta}
\]  
(7.7)

So
\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = \frac{d}{dt} \frac{\partial T}{\partial \dot{\theta}} = \frac{d}{dt} \left( \frac{1}{2} m r^2 \dot{\theta}^2 \right) = \frac{d}{dt} \left( m r^2 \dot{\theta} \right) = m r^2 \ddot{\theta}
\]  
(7.8)

and
\[
\frac{\partial L}{\partial \theta} = -\frac{\partial V}{\partial \theta} = \frac{\partial}{\partial \theta} \left( m g r \cos \theta \right) = -m g r \sin \theta
\]  
(7.9)

As a result, the EOM is
\[
m r^2 \ddot{\theta} = -m g r \sin \theta
\]  
(7.10)

\[
m r \dot{\theta} = -m g \sin \theta
\]  
(7.11)

which is the same as the second law of Newton:
\[
a = \frac{F}{m}
\]  
(7.12)

### 7.1.3. Hamiltonian, canonical coordinates and canonical momenta

From the Lagrangian, we can define a canonical momentum for every coordinate:
\[
p_i = \frac{\partial L}{\partial \dot{q}_i}
\]  
(7.13)

If the system has \(n\) coordinates, we will have \(n\) canonical momenta. If the coordinates we used are real space coordinates, these momenta coincide with the “momentum” we usually used in Newton’s theory. If the coordinates that we used here are angles, then the momenta will be angular momenta \(L\).

Hamiltonian:
\[
H = \sum p_i q_i - L = T + V
\]  
(7.14)

\(H\) is a function of \(p_i\) and \(q_i\)

For the pendulum example,
\[
p = \frac{\partial L}{\partial \dot{\theta}} = \frac{\partial T}{\partial \dot{\theta}} = \frac{\partial}{\partial \dot{\theta}} \left( \frac{1}{2} m r^2 \dot{\theta}^2 \right) = m r^2 \dot{\theta}
\]  
(7.15)

Notice that \(\dot{\theta}\) is just the angular velocity \(\omega\). Here, this \(p\) is in fact \(m r \omega\), i.e. the angular momentum.
\[
H = p \dot{\theta} - L = p \dot{\theta} - \frac{1}{2} m r \dot{\theta}^2 - m g r \cos \theta
\]  
(7.16)

Because \(p = m r^2 \dot{\theta}\), we can replace all \(\dot{\theta}\) by \(p/m r^2\)
\[
H = p \frac{p}{m r^2} - \frac{1}{2} m r^2 \left( \frac{p}{m r^2} \right)^2 - m g r \cos \theta = \frac{p^2}{m r^2} - \frac{p^2}{2 m r^2} - m g r \cos \theta = \frac{p^2}{2 m r^2} - m g r \cos \theta
\]  
(7.17)

This Hamiltonian is indeed a function of \(p\) and \(\theta\)

### 7.1.4. Canonical quantization

In a quantum system, all physical observable becomes quantum operators, including \(H, q_i\) and \(p_i\). The relation between them remains the same as in classical mechanics. The only ingredient that we need to add here is the “uncertainty relation”:
\[
[q_i, p_j] = i \hbar \delta_{i,j}
\]  
(7.18)
\[ [q_i, q_j] = [p_i, p_j] = 0 \]  
(7.19)
i.e., we request a coordinate NOT to commute with its canonical momentum. The commutator is assumed to be a constant, \( i\hbar \) for any canonical pair \( p_i \) and \( q_i \).

### 7.1.5. Summary

Step 1: starting from classical mechanics  
Step 2: define coordinates  
Step 3: find the canonical momenta for each coordinate  
Step 4: write down the Hamiltonian  
Step 5: require canonical commutation relation

**Example:** for the example we considered above, we have only one coordinate and one momentum, and the Hamiltonian looks like  
\[
H = \frac{p^2}{2mr^2} - mg r \cos \theta \]  
(7.20)

When we quantize this system, we turn everything into quantum operators  
\[
\hat{H} = \frac{\hat{p}^2}{2mr^2} - mg r \cos \hat{\theta} \]  
(7.21)

And we request \([\hat{q}, \hat{p}] = i\hbar\).  
Q: What is a \( \cos \) function of a quantum operator?  
A: We use Taylor expansions  
\[
\cos x = 1 - \frac{x^2}{2} + \frac{x^4}{24} + \ldots \]  
(7.22)

So  
\[
\cos \hat{\theta} = 1 - \frac{\hat{\theta}^2}{2} + \frac{\hat{\theta}^4}{24} + \ldots \]  
(7.23)

And thus  
\[
\hat{H} = \frac{\hat{p}^2}{2mr^2} - mg r \cos \hat{\theta} = \frac{\hat{p}^2}{2mr^2} - mg r \frac{\hat{\theta}^2}{2} + \frac{mg r}{24} \hat{\theta}^4 + \ldots \]  
(7.24)

We know that a constant in energy is not important, so we can drop the constant part \(-mg r\)  
\[
\hat{H} = \frac{\hat{p}^2}{2mr^2} - mg r \cos \hat{\theta} = \frac{\hat{p}^2}{2mr^2} + \frac{mg r}{2} \hat{\theta}^2 - \frac{mg r}{24} \hat{\theta}^4 + \ldots \]  
(7.25)

The first two terms here are the Hamiltonian of a harmonic oscillator. And the rest part of the Hamiltonian is known as the non-harmonic part of the potential.

### 7.2. Creation and annihilation operators

Q: How do we handle such a quantum system?  
A: By defining creation and annihilation operators.

#### 7.2.1. Creation and annihilation operators.

Define:
\[ a_i^+ = \frac{\sqrt{x} \, q_i - \frac{i}{\sqrt{x}} \, p_i}{\sqrt{2 \, \hbar}} \]  
(7.26)

\[ a_i = \frac{\sqrt{x} \, q_i + \frac{i}{\sqrt{x}} \, p_i}{\sqrt{2 \, \hbar}} \]  
(7.27)

where \( x \) is some arbitrary (positive) real number. It is easy to prove that \( a_i^\dagger \) and \( a_i^\dagger \) are conjugate of each other,

\[ (a_i^\dagger)^\dagger = a_i \]  
(7.28)

and it is easy to verify that [\( a_i, a_j \dagger \)] = 1

\[ a_i a_j^\dagger a_j = [a_i, a_j^\dagger] = \left[ \frac{\sqrt{x} \, q_i + \frac{i}{\sqrt{x}} \, p_i}{\sqrt{2 \, \hbar}}, \frac{\sqrt{x} \, q_i - \frac{i}{\sqrt{x}} \, p_i}{\sqrt{2 \, \hbar}} \right] = \frac{x}{2 \, \hbar} [q_i, q_j] + \frac{i}{2 \, \hbar} [p_i, q_j] - \frac{i}{2 \, \hbar} [q_j, p_i] + \frac{1}{2 \, \hbar} [p_j, p_i] = -i \frac{\hbar}{2 \, \hbar} = 1 \]  
(7.29)

More generally, we can prove that

\[ [a_i, a_j^\dagger] = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \]  
(7.30)

For the example that we considered above, there is only one coordinate and one momentum, \( q \) and \( p \), and thus, we only have one creation operator and one annihilation operator

\[ a^\dagger = \frac{\sqrt{x} \, q - \frac{i}{\sqrt{x}} \, p}{\sqrt{2 \, \hbar}} \]  
(7.31)

\[ a = \frac{\sqrt{x} \, q + \frac{i}{\sqrt{x}} \, p}{\sqrt{2 \, \hbar}} \]  
(7.32)

### 7.2.2. Vacuum

For simplicity, from now on, we will only focus on the example that discussed above, but please keep in mind that all conclusions can be generalized easily to more complicated Hamiltonians.

Here we make two assumptions:

**Assumption #1:** there is one (and only one) quantum state such that

\[ a \mid 0 \rangle = 0 \]  
(7.33)

We call this state the vacuum state.

**Assumption #2:** The states \( \mid 0 \rangle, a^\dagger \mid 0 \rangle, a^\dagger a^\dagger \mid 0 \rangle, a^\dagger a^\dagger a^\dagger \mid 0 \rangle \ldots \) form a complete basis of the Hilbert space.

Comment: These assumptions turn out to be true for most cases that we study in quantum mechanics.

### 7.2.3. Particle number operator

Define particle number operator

\[ n = a^\dagger a \]  
(7.34)

We can easily prove that this operator is a Hermitian operator, \( n^\dagger = n \)

\[ n^\dagger = (a^\dagger a^\dagger)^\dagger = a^\dagger (a^\dagger)^\dagger = a^\dagger a = n \]  
(7.35)
So this operator has real eigenvalues (which could be a physics measurable quantity).

We can further prove that

\[ n |0\rangle = a^\dagger a |0\rangle = a^\dagger (a |0\rangle) = a^\dagger x 0 = 0 \]  

(7.36)

i.e. the vacuum state \(|0\rangle\) is an eigenstate of \(n\) with eigenvalue 0

\[ n (a^\dagger |0\rangle) = a^\dagger a a^\dagger |0\rangle = a^\dagger (a a^\dagger - a^\dagger a + a^\dagger a) |0\rangle = a^\dagger (a^\dagger a |0\rangle + a^\dagger a |0\rangle + a^\dagger a |0\rangle) = a^\dagger |0\rangle \]  

(7.37)

The last term is 0, because \(a |0\rangle = 0\) by definition.

In other words, we find that \((a^\dagger)^m |0\rangle\) is also an eigenstate of \(n\) with eigenvalue 1.

Bottom line #1: the eigenvalues of the operator \(n\) is a non-negative integer 0, 1, 2, … Notice that number of particles are also non-negative integers, so it makes sense to call this operator the particle number operator. Here, the operator \(n\) measures the number of some fictitious particles

Bottom line #2: \((a^\dagger)^m |0\rangle\) with \(m\) being 0, 1, 2, … for a complete basis of the Hilbert space (as assumed above). Each state in this basis is an eigenstate of \(n\).

7.2.4. Hamiltonian: the harmonic part

\[ \hat{H} = \frac{\hat{p}^2}{2 m r^2} - m g r \cos \hat{q} = \frac{\hat{p}^2}{2 m r^2} + \frac{m g r}{2} \hat{q}^2 - \frac{m g r}{24} \hat{q}^4 + \ldots \]  

(7.38)

Let's keep only the first two terms, and ignore all higher order terms of \(\hat{q}\)

\[ \hat{H}_0 = \frac{\hat{p}^2}{2 m r^2} + \frac{m g r}{2} \hat{q}^2 \]  

(7.39)

The part that we ignored are

\[ \delta \hat{H} = -\frac{m g r}{24} \hat{q}^4 + \ldots \]  

(7.40)

and \(H = H_0 + \delta H\)

For the harmonic part \(H_0\)

\[ \hat{H}_0 = \frac{\hat{p}^2}{2 m r^2} + \frac{m g r}{2} \hat{q}^2 \]  

(7.41)

Because

\[ a^\dagger = \frac{\sqrt{x} q - \frac{1}{\sqrt{x}} i \hat{p}}{\sqrt{2 \hbar}} \]  

(7.42)

\[ a = \frac{\sqrt{x} q + \frac{1}{\sqrt{x}} i \hat{p}}{\sqrt{2 \hbar}} \]  

(7.43)

we know that

\[ q = \frac{\sqrt{\hbar}}{\sqrt{2 x}} (a^\dagger + a) \]  

(7.44)

\[ p = i \sqrt{\frac{x \hbar}{2}} (a^\dagger - a) \]  

(7.45)
Thus,

$$\hat{H}_0 = \frac{\hbar^2}{2m r^2} + \frac{mgr}{2} \hat{q}^2 = \frac{1}{2} \sqrt{\frac{\hbar}{2}} (a^\dagger - a)^2 + \frac{mgr}{2} \left( \frac{\sqrt{\hbar}}{\sqrt{2x}} (a^\dagger + a)^2 \right)^2 = -\frac{\hbar}{4x} (a^\dagger - a)^2 + \frac{mgr}{4x} (a^\dagger + a)^2.$$  (7.46)

Here

$$(a^\dagger - a)^2 = (a^\dagger - a)(a^\dagger - a) = a^\dagger a^\dagger - a^\dagger a - a a^\dagger + a a$$  (7.47)

and

$$(a^\dagger + a)^2 = (a^\dagger + a)(a^\dagger + a) = a^\dagger a^\dagger + a^\dagger a + a a^\dagger + a a$$  (7.48)

So

$$\hat{H}_0 = \left(-\frac{xh}{4m r^2} + \frac{mgrh}{4x}\right)(a^\dagger a^\dagger + a a) + \left(\frac{xh}{4m r^2} + \frac{mgrh}{4x}\right)(a^\dagger + a^\dagger a)$$  (7.49)

Now, we choose the value of $x$, such that the first term vanish

$$-\frac{xh}{4m r^2} + \frac{mgrh}{4x} = 0$$  (7.50)

i.e.

$$x^2 = m^2 gr^3$$  (7.51)

$$x = \sqrt{m^2 gr^3} = m r \sqrt{gr}$$  (7.52)

And thus

$$\hat{H}_0 = \left(-\frac{xh}{4m r^2} + \frac{mgrh}{4x}\right)(a^\dagger a^\dagger + a a) + \left(\frac{xh}{4m r^2} + \frac{mgrh}{4x}\right)(a^\dagger + a^\dagger a) =$$

$$= \frac{h}{4m r^2} (a^\dagger a + a^\dagger a)$$  (7.53)

Because $[a, a^\dagger] = a a^\dagger - a^\dagger a = 1$, $a a^\dagger = a^\dagger a + 1$ and thus

$$\hat{H}_0 = h \sqrt{g/r} \left(\frac{a^\dagger a + a^\dagger a}{2}\right) = h \sqrt{g/r} \left(\frac{a^\dagger a + a^\dagger a + 1}{2}\right) = h \sqrt{g/r} \left(\frac{2a^\dagger a + 1}{2}\right) = h \sqrt{g/r} \left(\frac{a^\dagger a + 1}{2}\right)$$  (7.54)

Notice that $\sqrt{g/r}$ is actually the angular frequency of the harmonic oscillator, and $a^\dagger a$ is in fact the particle number operator $n$ we defined above

$$\hat{H}_0 = h \omega \left(n + \frac{1}{2}\right)$$  (7.55)

We can understand this Hamiltonian as the following: (1) each of our fictitious particle has energy $\hbar \omega$. (2) The system also have an zero point energy (energy of the vacuum) $\hbar \omega$. So the total energy of the system is

$$\hat{H}_0 = h \omega \left(n + \frac{1}{2}\right)$$  (7.56)

Because the energy is carried by these fictitious particles, the total energy is proportional to particle number (up to the zero point energy $\hbar \omega/2$). Because particle number are quantized integers, the energy is quantized.

This is the origin of quantization
7.2.5. Hamiltonian: the non-harmonic part

How about the terms that we ignored?

We can treat them as interactions between particles (i.e. scatterings).

The bottom line:

1) for a harmonic oscillator, we can treat it as non-interacting particles (each has energy $\hbar \omega$)

2) for non-harmonic terms, we can treat term as interactions between these particles

7.2.6. How about waves?

For a harmonic oscillator, we know that we can think about it using these fictitious particles. This fictitious particles cannot move (they are confined spatially at the oscillator). This is a bit different from a real particle, which can move in space. How can we have a real particle? Using waves, instead of a single oscillator.

Waves is nothing but couple harmonic oscillators (we put a harmonic oscillator at each position $x$, and couple them together). For each position $x$, we have one harmonic oscillator, and thus we can define a creation operator at this point $a^\dagger(x)$ and also an annihilation operator $a(x)$ at this point.

We can also ask what is the particle number for each oscillator $n(x) = a^\dagger(x) a(x)$

The coupling between harmonic oscillators allows the particle at $x$ to move to $y$ (i.e. motion of a particle).

Non-harmonic parts gives interactions between this particles.

This is the foundation of particle wave duality.