221B Lecture Notes

Quantum Field Theory (a.k.a. Second Quantization)

1 Quantum Field Theory

Why quantum field theory? We know quantum mechanics works perfectly well for many systems we had looked at already. Then why go to a new formalism? The following few sections describe motivation for the quantum field theory, which I introduce as a re-formulation of multi-body quantum mechanics with identical physics content.

1.1 Limitations of Multi-body Schrödinger Wave Function

We used totally anti-symmetrized Slater determinants for the study of atoms, molecules, nuclei. Already with the number of particles in these systems, say, about 100, the use of multi-body wave function is quite cumbersome. Mention a wave function of an Avogardro number of particles! Not only it is completely impractical to talk about a wave function with 6×10^{23} coordinates for each particle, we even do not know if it is supposed to have 6×10^{23} or $6 \times 10^{23} + 1$ coordinates, and the property of the system of our interest shouldn't be concerned with such a tiny (?) difference.

Another limitation of the multi-body wave functions is that it is incapable of describing processes where the number of particles changes. For instance, think about the emission of a photon from the excited state of an atom. The wave function would contain coordinates for the electrons in the atom and the nucleus in the initial state. The final state contains yet another particle, photon in this case. But the Schrödinger equation is a differential equation acting on the arguments of the Schrödinger wave function, and can never change the number of arguments. Similarly, it is useful to consider elementary excitations in multi-body systems, such as phonons, and they can be created or annihilated by putting energy into the system. Finally even the number of matter particles changes in relativistic elementary paticle physics by pair creations, pair annihilations etc.

The limitaions of multi-body Schrödinger wave function mentioned here call for a better formalism. The quantum field theory is designed specifically for that. But before talking about quantum field theory, let us first discuss classical field theory.

1.2 Aim of the Quantum Field Theory

Quantum Field Theory is sometimes called "2nd quantization." This is a very bad misnomer because of the reason I will explain later. But nonetheless, you are likely to come across this name, and you need to know it.

The aim of the quantum field theory is to come up with a formalism which is completely equivalent to multi-body Schrödinger equations but just better: it allows you to consider a variable number of particles all within the same framework and can even describe the change in the number of particles. It also gives totally symmetric or anti-symmetric multi-body wave function automatically, not as a consequence of symmetrization or anti-symmetrization done "by hand." Moreover, once we go to relativistic systems, quantum field theory is the only known formalism to describe quantum mechanics consistent with Lorentz invariance and causality. It also allows a systematic way of organizing perturbation theory in terms of "Feynman diagrams," a graphical representation of each term in perturbation theory.

Even though the contents of multi-body quantum mechanics and quantum field theory are exactly the same in systems where the number of particles does not change, it turns out that the field theory is a far better formalism for many purposes and is widely used in condensed matter physics, elementary particle physics, quantum optics, and in some cases also in atomic/molecular physics and nuclear physics. It is particularly suited to multi-body problems. In systems where the number of particles changes, or where one needs superposition of states with different number of particles (sounds odd, but we will see examples later), quantum field theory is crucial.

But it is clear that the formalism will confuse you (at least) once because of too-close resemblance but conceptual difference from the ordinary Schrödinger equation. I will try to make it as clear as possible below.

1.3 Particle-Wave Duality

It is interesting to note that the way quantum mechanics and quantum field theory work is a sort of the opposite. In quantum mechanics, you start with classical particle Hamiltonian mechanics, with no concept of wave or interference. After quantizing it, we introduce Schrödinger wave function and there emerges concepts of wave and its interference. In quantum field theory, you start with classical wave equation, with no concept of particle. After quantizing it, we find particle interpretation of excitations in the system. Either way, we find particle-wave duality, *i.e.*, the energy/momentum is carried by a quantum object which is neither exactly a wave or a particle. It is both. Nonetheless, two formalisms start from the opposite classical description and arrive at the same conclusion.

2 Classical Schrödinger Field

Let us consider a *classical* field equation

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \Delta}{2m} \right) \psi(\vec{x}, t) = 0. \tag{1}$$

This looks just like quantum mechanical Schrödinger equation, but we consider it as a classical field equation similar to the Maxwell equation in Electromagnetism. You may wonder why there is $\hbar$ in the equation, then. I can actually eliminate $\hbar$ completely from the equation by introducing a new quantities $\mu = m/\hbar$. For a later convenience when we discuss the action of the classical Schrödinger field, let me also introduce $\phi = \hbar^{1/2}\psi$. Then the field equation is

$$\left(i\frac{\partial}{\partial t} + \frac{\Delta}{2\mu} \right) \phi(\vec{x}, t) = 0. \tag{2}$$

There is no trace of $\hbar$ any more. Of course, the parameter μ has a dimension of $L^{-2}T$ and does not have a meaning as a "mass" of a particle. But we are talking about a classical field equation, and there is no concept of a "mass" in a classical field equation anyway. μ is just a parameter in the field equation. A solution to this field equation is that of a plane wave

$$\phi(\vec{x}, t) = e^{i\vec{k}\cdot\vec{x} - i\omega t}, \tag{3}$$

where the angular frequency ω and the wave vector $\vec{k}$ are related as

$$\omega = \frac{\vec{k}^2}{2\mu}. \tag{4}$$

You can see that the parameter μ defines the dispersion relation between the frequency and the wave vector.

This classical field equation can be derived from the action

$$S = \int d\vec{x} dt \phi^*(\vec{x}, t) \left(i \frac{\partial}{\partial t} + \frac{\Delta}{2\mu} \right) \phi(\vec{x}, t). \tag{5}$$

Note that the Lagrangian for a field is given by an integral over space, and in this case

$$S = \int dt L(t) = \int dt \vec{x} \mathcal{L}(\vec{x}, t) \tag{6}$$

where $\mathcal{L}(\vec{x}, t)$ is called Lagrangian density. By taking the variation of the action with respect to $\phi^* \to \phi^* + \delta\phi^*$, we find

$$\delta S = \int d\vec{x} dt \delta\phi^*(\vec{x}, t) \left(i \frac{\partial}{\partial t} + \frac{\Delta}{2\mu} \right) \phi(\vec{x}, t), \tag{7}$$

and requiring that the action must be stationary, we recover the field equation Eq. (2). You may worry that the action Eq. (5) is not real; but it can be made real by adding surface terms

$$S = \int d\vec{x} dt \left(\frac{i}{2} (\phi^* \dot{\phi} - \dot{\phi}^* \phi) - \frac{1}{2\mu} \vec{\nabla} \phi^* \vec{\nabla} \phi \right). \tag{8}$$

But for simplicity we use the previous form Eq. (5) for the rest of the note.

Because the classical field theory does not need to be linear unlike quantum mechanical Schrödinger equation, we can add a non-linear term (higher than quadratic term) in the action, for instance,

$$S = \int d\vec{x} dt \left(i \phi^* \dot{\phi} + \phi^* \frac{\Delta}{2\mu} \phi - \frac{1}{2} \gamma \phi^{*2} \phi^2 \right). \tag{9}$$

The parameter γ has a dimension of $M^{-1}L$. Following the same variation, we find a non-linear field equation

$$\left(i \frac{\partial}{\partial t} + \frac{\Delta}{2\mu} - \gamma \phi^* \phi \right) \phi(\vec{x}, t) = 0. \tag{10}$$

This equation is non-linear and we cannot solve this equation exactly in general any more.

3 Quick Review of Quantization Procedure

Let us briefly review how we quantize a particle mechanics system. Given an action on the phase space (p_i, q_i),

$$S = \int dt L = \int dt (\sum_i p_i \dot{q}_i - H(p_i, q_j)), \tag{11}$$

the variational principle gives the Hamilton equations of motion

$$\frac{\delta S}{\delta p_i} = \dot{q}_i - \frac{\partial H}{\partial p_i} = 0, \tag{12}$$

$$\frac{\delta S}{\delta q_i} = -\dot{p}_i - \frac{\partial H}{\partial q_i} = 0. \tag{13}$$

You can again add a surface term and make it look symmetric between p and q as $L = \sum_i \frac{1}{2}(p_i \dot{q}_i - q_i \dot{p}_i) - H(p, q)$. To quantize this system, we first identify the canonically conjugate momentum of the coordinate q_i by

$$p_i = \frac{\partial L}{\partial \dot{q}_i}. \tag{14}$$

Then we set up the canonical commutation relation

$$[p_i, p_j] = [q_i, q_j] = 0, \qquad [p_i, q_j] = -i\hbar \delta_{ij}. \tag{15}$$

This defines the quantum theory. The index i runs over all degrees of freedom in the system. The quantum mechanical state is given by a ket $|\psi(t)\rangle$, which admits a "coordinate representation" $\langle q|\psi\rangle = \psi(q, t)$. The dynamical evolution of the system is given by the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(p_i, q_j)|\psi(t)\rangle. \tag{16}$$

It is also useful to recall the commutation relation between creation and annihilation operator of harmonic oscillators

$$[a_i, a_j^\dagger] = \delta_{ij}, \qquad [a, a] = [a^\dagger, a^\dagger] = 0. \tag{17}$$

Here, I assumed there are many harmonic oscillators labeled by the subscript i or j. The Hilbert space is constructed from the ground state $|0\rangle$ which satisfies

$$a_i|0\rangle = 0 \tag{18}$$

for all i. All other states are given by acting creation operators on the ground state

$$|n_1, n_2, \cdots, n_N\rangle = \frac{1}{\sqrt{n_1! n_2! \cdots n_N!}} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \cdots (a_N^\dagger)^{n_N} |0\rangle \tag{19}$$

We will use the same method to construct Hilbert space for the quantized Schrödinger field.

4 Quantized Schrödinger Field

Now we try to quantize the classical field theory given by the action Eq. (9). The procedure is the same as in particle mechanics, except that the index i that runs over all degrees of freedom is now replace by $\vec{x}$. What it means is that $\vec{x}$ is not an operator (!) but merely an index. This is probably one of the most confusing points about the field theory. $\phi(\vec{x})$ at different positions are regarded as independent canonical coordinates exactly in the same way that q_i with different i are regarded as independent canonical coordinates in particle mechanics.

4.1 Canonical Commutation Relation

The canonically conjugate momenta $\pi(\vec{x})$ of the canonical coordinates $\psi(\vec{x})$ is obtained from Eq. (9) in the same way as in Eq. (14), namely

$$\pi(\vec{x}) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(\vec{x})} = i\phi^*(\vec{x}). \tag{20}$$

We will use $\phi^\dagger$ below instead of ϕ^* because it is more common notation for complex conjugates (hermitean conjugates) for operators. Note that we regard the integration over space $\vec{x}$ in the Lagrangian a generalization of the summation over the index i in Eq. (11).

Given the canonical coordinates $\phi(\vec{x})$ and canonical momenta $\pi(\vec{x})$, we introduce canonical commutation relation

$$[\pi(\vec{x}), \phi(\vec{y})] = [i\phi^\dagger(\vec{x}), \phi(\vec{y})] = -i\hbar\delta(\vec{x} - \vec{y}). \tag{21}$$

The delta function is a generalization of the Kronecker's delta in Eq. (15).

This defines the quantum theory of the Schrödinger field.[1] The canonical commutation relation Eq. (21) is very similar to the case of the harmonic oscillator. We now go back to the operator $\psi(\vec{x}) = \phi(\vec{x})/\hbar^{1/2}$, and we find

$$[\psi(\vec{x}), \psi^\dagger(\vec{y})] = \delta(\vec{x} - \vec{y}), \qquad [\psi, \psi] = [\psi^\dagger, \psi^\dagger] = 0, \tag{22}$$

which resembles the case of harmonic oscillator even better. Now you see that the use of $\psi(\vec{x})$ was more convenient (we are not afraid of having $\hbar$ in the Lagrangian any more because we are discussing a quantum theory anyway). We now regard $\psi(\vec{x})$ as annihilation operator and $\psi^\dagger(\vec{x})$ creation operator of a particle at position $\vec{x}$.

The Hamiltonian of the system from the action Eq. (9) is read off in the same way as in Eq. (11):

$$H = \int d\vec{x} \left(\phi^\dagger \frac{-\Delta}{2\mu} \phi + \frac{1}{2} \gamma (\phi^\dagger \phi)^2 \right) = \int d\vec{x} \left(\psi^\dagger \frac{-\hbar^2 \Delta}{2m} \psi + \frac{1}{2} \hbar^2 \gamma \psi^{\dagger 2} \psi^2 \right). \tag{23}$$

Here I recovered $m = \hbar \mu$. Note that

$$H|0\rangle = 0 \tag{24}$$

because $\psi(\vec{x})$ in the Hamiltonian annihilates directly the vacuum. A general state must satisfy the Schrödinger equation in the same way as in particle mechanics

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle \tag{25}$$

It is useful for later purpose to calculate the commutator $[H, \psi^\dagger(\vec{x})]$.

$$\begin{aligned} [H, \psi^\dagger(\vec{x})] &= \int d\vec{y} [\left(\psi^\dagger(\vec{y}) \frac{-\hbar^2 \Delta_{\vec{y}}}{2m} \psi(\vec{y}) + \frac{1}{2} \hbar^2 \gamma \psi^{\dagger 2}(\vec{y}) \psi(\vec{y})^2 \right), \psi^\dagger(\vec{x})] \\ &= \left(\frac{-\hbar^2 \Delta_{\vec{x}}}{2m} \psi^\dagger(\vec{x}) + \frac{1}{2} \hbar^2 \gamma \psi^{\dagger 2}(\vec{x}) 2 \psi(\vec{x}) \right). \end{aligned} \tag{26}$$

[1] The commutation relation is given in the Schrödinger picture, where the operators do not evolve in time while the states do. When switching to Heisenberg picture, we have to specify that the canonical commutation relation holds only at equal times: $[\pi(\vec{x}, t), \phi(\vec{y}, t)] = [i\phi^\dagger(\vec{x}, t), \phi(\vec{y}, t)] = -i\hbar \delta(\vec{x} - \vec{y})$. Commutation relation of operators at unequal times would depend on the dynamics of the system.

4.2 Fock Space

The canonical commutation relation Eq. (21) allows us to construct the Hilbert space following the experience of the harmonic oscillator. The particular Hilbert space we construct below is called Fock space.

We define the "vacuum" $|0\rangle$ which is annihilated by the annihilation operator

$$\psi(\vec{x})|0\rangle = 0, \tag{27}$$

and construct the Fock space by

$$|\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N\rangle = \psi^\dagger(\vec{x}_1)\psi^\dagger(\vec{x}_2)\cdots\psi^\dagger(\vec{x}_N)|0\rangle. \tag{28}$$

You can use $(\psi(\vec{x}_1))^{n_1}$ as well, but we will not need it for the later discussions.

What is the physical meaning of the Fock space we have constructed? It turns out that the state $|\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_n\rangle$ in Eq. (28) has a very simple meaning: it is an n-particle state of identical bosons in the position eigenstate at $\vec{x}_1, \cdots, \vec{x}_n$. We will verify this interpretation below explicitly.

4.3 One-particle State

Let us first study the one-particle state

$$|\vec{x}\rangle = \psi^\dagger(\vec{x})|0\rangle. \tag{29}$$

The first quantity we calculate is its norm. Here we go:

$$\begin{aligned}
\langle\vec{x}|\vec{y}\rangle &= \langle 0|\psi(\vec{x})\psi^\dagger(\vec{y})|0\rangle \\
&= \langle 0|[\psi(\vec{x}), \psi^\dagger(\vec{y})]|0\rangle \\
&= \langle 0|\delta(\vec{x}-\vec{y})0\rangle \\
&= \delta(\vec{x}-\vec{y}).
\end{aligned} \tag{30}$$

Therefore, this state is normalized in the same way as the one-particle position eigenstate.

A general one-particle state is a superposition of position eigenstates. We define a general state

$$|\Psi(t)\rangle = \int d\vec{x}\Psi(\vec{x},t)|\vec{x}\rangle = \int d\vec{x}\Psi(\vec{x})\psi^\dagger(\vec{x})|0\rangle. \tag{31}$$

Note that $\Psi(\vec{x})$ is a c-number function which determines a particular superposition of the position eigenstates $|\vec{x}\rangle$. But it turns out that this $\Psi(\vec{x})$

corresponds to the Schrödinger wave function in the particle quantum mechanics. This can be seen by using the Schrödinger equation Eq. (25) with the Hamiltonian Eq. (23) and the state Eq. (29). The l.h.s of the Schrödinger equation is then

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \int d\vec{x}\left(i\hbar\frac{\partial}{\partial t}\Psi(\vec{x},t)\right)|\vec{x}\rangle. \tag{32}$$

On the other hand, the r.h.s of the Schrödinger equation is

$$\begin{aligned}
H|\Psi(t)\rangle &= \int d\vec{x}\Psi(\vec{x})H\psi^\dagger(\vec{x})|0\rangle \\
&= \int d\vec{x}\Psi(\vec{x})[H,\psi^\dagger(\vec{x})]|0\rangle \\
&= \int d\vec{x}\left(\frac{-\hbar^2\Delta_{\vec{x}}}{2m}\psi^\dagger(\vec{x}) + \frac{1}{2}\hbar^2\gamma\psi^{\dagger 2}(\vec{x})2\psi(\vec{x})\right)\Psi(\vec{x},t)|0\rangle \\
&= \int d\vec{x}\left(\frac{-\hbar^2\Delta_{\vec{x}}}{2m}\Psi(\vec{x},t)\right)\psi^\dagger(\vec{x})|0\rangle \\
&= \int d\vec{x}\left(\frac{-\hbar^2\Delta}{2m}\Psi(\vec{x},t)\right)|\vec{x}\rangle. \qquad (33)
\end{aligned}$$

Comparing Eqs. (32,33), we find

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{x},t) = \frac{-\hbar^2\Delta}{2m}\Psi(\vec{x},t) \tag{34}$$

which is nothing but a Schrödinger equation for a free one-particle wave function $\Psi(\vec{x},t)$. Therefore, the Fock space with a single creation operator correctly describes the one-particle particle mechanics.

4.4 Two-Particle State

Let us next study the two-particle state

$$|\vec{x}_1,\vec{x}_2\rangle = \frac{1}{\sqrt{2}}\psi^\dagger(\vec{x}_1)\psi^\dagger(\vec{x}_2)|0\rangle. \tag{35}$$

The first quantity we calculate is again its norm. Here we go:

$$\langle\vec{x}_1,\vec{x}_2|\vec{y}_1,\vec{y}_2\rangle = \frac{1}{2}\langle 0|\psi(\vec{x}_2)\psi(\vec{x}_1)\psi^\dagger(\vec{y}_1)\psi^\dagger(\vec{y}_2)|0\rangle$$

$$= \frac{1}{2}\langle 0|\psi(\vec{x}_2)([\psi(\vec{x}_1), \psi^\dagger(\vec{y}_1)] + \psi^\dagger(\vec{y}_1)\psi(\vec{x}_1))\psi^\dagger(\vec{y}_2)|0\rangle$$
$$= \frac{1}{2}\langle 0|\psi(\vec{x}_2)\delta(\vec{x}_1 - \vec{y}_1)\psi^\dagger(\vec{y}_2) + \psi(\vec{x}_2)\psi^\dagger(\vec{y}_1)\psi(\vec{x}_1))\psi^\dagger(\vec{y}_2)|0\rangle$$
$$= \frac{1}{2}\langle 0|\delta(\vec{x}_1 - \vec{y}_1)[\psi(\vec{x}_2), \psi^\dagger(\vec{y}_2)] + [\psi(\vec{x}_2), \psi^\dagger(\vec{y}_1)][\psi(\vec{x}_1)), \psi^\dagger(\vec{y}_2)]|0\rangle$$
$$= \frac{1}{2}\left(\delta(\vec{x}_1 - \vec{y}_1)\delta(\vec{x}_2 - \vec{y}_2) + \delta(\vec{x}_1 - \vec{y}_2)\delta(\vec{x}_2 - \vec{y}_1)\right). \quad (36)$$

This normalization suggests that we are dealing with a two-particle state of identical particles, because the norm is non-vanishing when $\vec{x}_1 = \vec{y}_1$ and $\vec{x}_2 = \vec{y}_2$, but also when $\vec{x}_1 = \vec{y}_2$ and $\vec{x}_2 = \vec{y}_1$, *i.e.*, two particles interchanged.

A general two-particle state is given by

$$|\Psi(t)\rangle = \int d\vec{x}_1 d\vec{x}_2 \Psi(\vec{x}_1, \vec{x}_2, t)|\vec{x}_1, \vec{x}_2\rangle = \frac{1}{\sqrt{2}}\int d\vec{x}_1 d\vec{x}_2 \Psi(\vec{x}_1, \vec{x}_2)\psi^\dagger(\vec{x}_1)\psi^\dagger(\vec{x}_2)|0\rangle. \quad (37)$$

Because $[\psi^\dagger(\vec{x}_1), \psi^\dagger(\vec{x}_2)] = 0$, the integration over $\vec{x}_1$ and $\vec{x}_2$ is symmetric under the interchange $\vec{x}_1 \leftrightarrow \vec{x}_2$, and hence $\Psi(\vec{x}_1, \vec{x}_2, t) = \Psi(\vec{x}_2, \vec{x}_1, t)$. The symmetry under the exchange suggests that we are dealing with identical bosons.

The fact that we see two identical particles becomes clearer by again working out the time evolution of a general state. Using the Schrödinger equation Eq. (25) with the Hamiltonian Eq. (23) and the state Eq. (35), the l.h.s of the Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \int d\vec{x}_1 d\vec{x}_2 \left(i\hbar\frac{\partial}{\partial t}\Psi(\vec{x}_1, \vec{x}_2, t)\right)|\vec{x}_1, \vec{x}_2\rangle. \quad (38)$$

On the other hand, the r.h.s of the Schrödinger equation is

$$\sqrt{2}H|\Psi(t)\rangle = \int d\vec{x}_1 d\vec{x}_2 \Psi(\vec{x}_1, \vec{x}_2, t)H\psi^\dagger(\vec{x}_1)\psi^\dagger(\vec{x}_2)|0\rangle$$
$$= \int d\vec{x}_1 d\vec{x}_2 \Psi(\vec{x}_1, \vec{x}_2, t)([H, \psi^\dagger(\vec{x}_1)] + \psi^\dagger(\vec{x}_1)H)\psi^\dagger(\vec{x}_2)|0\rangle$$
$$= \int d\vec{x}_1 d\vec{x}_2 \left(\frac{-\hbar^2\Delta_{\vec{x}_1}}{2m}\psi^\dagger(\vec{x}_1) + \frac{1}{2}\hbar^2\gamma\psi^{\dagger 2}(\vec{x}_1)2\psi(\vec{x}_1)\right)\Psi(\vec{x}_1, \vec{x}_2, t)\psi^\dagger(\vec{x}_2)|0\rangle$$
$$+ \int d\vec{x}_1 d\vec{x}_2 \Psi(\vec{x}_1, \vec{x}_2, t)\psi^\dagger(\vec{x}_1)[H, \psi^\dagger(\vec{x}_2)]|0\rangle$$
$$= \int d\vec{x}\left(\psi^\dagger(\vec{x}_1)\frac{-\hbar^2\Delta_{\vec{x}_1}}{2m} + \hbar^2\gamma\psi^{\dagger 2}(\vec{x}_1)\psi(\vec{x}_1)\right)\Psi(\vec{x}_1, \vec{x}_2, t)\psi^\dagger(\vec{x}_2)|0\rangle$$

$$
\begin{aligned}
&+\int d\vec{x}_1 d\vec{x}_2 \psi^\dagger(\vec{x}_1)\left(\frac{-\hbar^2\Delta_{\vec{x}_2}}{2m}\psi^\dagger(\vec{x}_2)+\frac{1}{2}\hbar^2\gamma\psi^{\dagger 2}(\vec{x}_2)2\psi(\vec{x}_2)\right)\Psi(\vec{x}_1,\vec{x}_2,t)|0\rangle \\
&=\sqrt{2}\int d\vec{x}_1 d\vec{x}_2\left(\frac{-\hbar^2\Delta_{\vec{x}_1}}{2m}+\frac{-\hbar^2\Delta_{\vec{x}_2}}{2m}+\hbar^2\gamma\delta(\vec{x}_1-\vec{x}_2)\right)\Psi(\vec{x}_1,\vec{x}_2,t)|\vec{x}_1,\vec{x}_2\rangle.
\end{aligned}
\tag{39}
$$

Comparing Eqs. (38,39), we find

$$
i\hbar\frac{\partial}{\partial t}\Psi(\vec{x}_1,\vec{x}_2,t)=\left(\frac{-\hbar^2\Delta_{\vec{x}_1}}{2m}+\frac{-\hbar^2\Delta_{\vec{x}_2}}{2m}+\hbar^2\gamma\delta(\vec{x}_1-\vec{x}_2)\right)\Psi(\vec{x}_1,\vec{x}_2,t) \tag{40}
$$

which is nothing but a Schrödinger equation for two-particle wave function $\Psi(\vec{x},t)$, with a delta function potential as an interaction between them. Therefore, the Fock space with two creation operators correctly describes the two-particle particle mechanics. If we want a general interaction potential between them, the action Eq. (9) must be modified to

$$
S=\int dt\left[\int d\vec{x}\left(\psi^* i\hbar\dot{\psi}+\psi^*\frac{\hbar^2\Delta}{2m}\psi\right)-\int d\vec{x}d\vec{y}\frac{1}{2}\psi^*(\vec{x})\psi^*(\vec{y})V(\vec{x}-\vec{y})\psi(\vec{y})\psi(\vec{x})\right]. \tag{41}
$$

The corresponding Hamiltonian is

$$
H=\int d\vec{x}\psi^*\frac{-\hbar^2\Delta}{2m}\psi+\int d\vec{x}d\vec{y}\frac{1}{2}\psi^*(\vec{x})\psi^*(\vec{y})V(\vec{x}-\vec{y})\psi(\vec{y})\psi(\vec{x}). \tag{42}
$$

You can follow exactly the same steps as above and derive the equation

$$
i\hbar\frac{\partial}{\partial t}\Psi(\vec{x}_1,\vec{x}_2,t)=\left(\frac{-\hbar^2\Delta_{\vec{x}_1}}{2m}+\frac{-\hbar^2\Delta_{\vec{x}_2}}{2m}+V(\vec{x}_1-\vec{x}_2)\right)\Psi(\vec{x}_1,\vec{x}_2,t). \tag{43}
$$

In summary, the quantized Schrödinger field correctly describes the two interacting identical bosons appropriately.

4.5 Three and More Particles

Following the same analysis as two-particle case, we can consider the three-particle state

$$
|\vec{x}_1,\vec{x}_2,\vec{x}_3\rangle=\frac{1}{\sqrt{3!}}\psi^\dagger(\vec{x}_1)\psi^\dagger(\vec{x}_2)\psi^\dagger(\vec{x}_3)|0\rangle, \tag{44}
$$

and its norm is given by

$$
\begin{aligned}
&\langle \vec{x}_1, \vec{x}_2, \vec{x}_3 | \vec{y}_1, \vec{y}_2, \vec{y}_3 \rangle \\
&\quad = \frac{1}{3!}(\delta(\vec{x}_1 - \vec{y}_1)\delta(\vec{x}_2 - \vec{y}_2)\delta(\vec{x}_3 - \vec{y}_3) + \delta(\vec{x}_1 - \vec{y}_2)\delta(\vec{x}_2 - \vec{y}_3)\delta(\vec{x}_3 - \vec{y}_1) \\
&\qquad + \delta(\vec{x}_1 - \vec{y}_3)\delta(\vec{x}_2 - \vec{y}_1)\delta(\vec{x}_3 - \vec{y}_2) + \delta(\vec{x}_1 - \vec{y}_2)\delta(\vec{x}_2 - \vec{y}_1)\delta(\vec{x}_3 - \vec{y}_3) \\
&\qquad + \delta(\vec{x}_1 - \vec{y}_3)\delta(\vec{x}_2 - \vec{y}_2)\delta(\vec{x}_3 - \vec{y}_1) + \delta(\vec{x}_1 - \vec{y}_1)\delta(\vec{x}_2 - \vec{y}_3)\delta(\vec{x}_3 - \vec{y}_2)).
\end{aligned} \tag{45}
$$

A general three-particle state is

$$
|\Psi(t)\rangle = \int d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 \Psi(\vec{x}_1, \vec{x}_2, \vec{x}_3, t) |\vec{x}_1, \vec{x}_2, \vec{x}_3\rangle. \tag{46}
$$

Using the Hamiltonian Eq. (42), the Schrodinger equation reduces to

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} \Psi(\vec{x}_1, \vec{x}_2, \vec{x}_3) = \bigg[&-\frac{\hbar^2 \Delta_{\vec{x}_1}}{2m} - \frac{\hbar^2 \Delta_{\vec{x}_2}}{2m} - \frac{\hbar^2 \Delta_{\vec{x}_3}}{2m} \\
&+ V(\vec{x}_1 - \vec{x}_2) + V(\vec{x}_1 - \vec{x}_3) + V(\vec{x}_2 - \vec{x}_3) \bigg] \Psi(\vec{x}_1, \vec{x}_2, \vec{x}_3).
\end{aligned} \tag{47}
$$

In general, an n-particle state can be constructed as

$$
|\Psi\rangle = \frac{1}{\sqrt{n!}} \int d\vec{x}_1 \cdots d\vec{x}_n \Psi(\vec{x}_1, \cdots, \vec{x}_n) \psi^\dagger(\vec{x}_1) \cdots \psi^\dagger(\vec{x}_n) |0\rangle. \tag{48}
$$

The symmetry of the wave function under interchange of any of the n particles is automatic, and hence it describes identical bosons.

4.6 The Number Operator

The total number of particles is an eigenvalue of the operator

$$
N = \int d\vec{x} \psi^\dagger(\vec{x}) \psi(\vec{x}). \tag{49}
$$

This is probably obvious from the analogy to the harmonic oscillator, but nonetheless let us prove it. First consider the commutators

$$
[N, \psi(\vec{x})] = \int d\vec{y} [\psi^\dagger(\vec{y})\psi(\vec{y}), \psi(\vec{x})] = \int d\vec{y} (-\delta(\vec{y} - \vec{x}))\psi(\vec{y}) = -\psi(\vec{x}), \tag{50}
$$

and also

$$[N,\psi^\dagger(\vec{x})] = \int d\vec{y}[\psi^\dagger(\vec{y})\psi(\vec{y}),\psi^\dagger(\vec{x})] = \int d\vec{y}\psi^\dagger(\vec{y})\delta(\vec{y}-\vec{x}) = \psi^\dagger(\vec{x}). \quad (51)$$

It is useful to rewrite this commutator as

$$N\psi^\dagger(\vec{x}) = \psi^\dagger(\vec{x})(N+1). \quad (52)$$

In other words, every time you change the order of the number operator N and the creation operator $\psi^\dagger$, N increases by one. Note also

$$N|0\rangle = 0, \quad (53)$$

because the annihilation operator in N acts directly on the vacuum. Then the eigenvalue of N on n-body state can be read off quite easily.

$$\begin{aligned} N|\vec{x}_1,\cdots,\vec{x}_n\rangle &= \frac{1}{\sqrt{n!}}N\psi^\dagger(\vec{x}_1)\cdots\psi^\dagger(\vec{x}_n)|0\rangle \\ &= \frac{1}{\sqrt{n!}}\psi^\dagger(\vec{x}_1)(N+1)\cdots\psi^\dagger(\vec{x}_n)|0\rangle \\ &= \cdots \\ &= \frac{1}{\sqrt{n!}}\psi^\dagger(\vec{x}_1)\cdots\psi^\dagger(\vec{x}_n)(N+n)|0\rangle \\ &= n|\vec{x}_1,\cdots,\vec{x}_n\rangle. \end{aligned} \quad (54)$$

We see that the operator N indeed picks up the number of the particles in a given state as its eigenvalue.

4.7 Momentum Space

It may be more intuitive to consider creation and annihilation operators in the momentum space, because the Hamiltonian is "diagonal" in the momentum space in the absence of the interaction potential.

Suppose that the whole system is in a cubic box of volume $V = L^3$ with a periodic boundary condition. This choice of the boundary condition is often called the "box normalization." Then the field operator can be expanded in the Fourier series

$$\psi(\vec{x}) = \frac{1}{L^{3/2}}\sum_{\vec{p}} a(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar}, \quad (55)$$

where

$$\vec{p} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z) \tag{56}$$

with integer $n_{x,y,z}$. The inverse transform is therefore

$$a(\vec{p}) = \frac{1}{L^{3/2}} \int d\vec{x} \psi(\vec{x}) e^{-i\vec{p}\cdot\vec{x}/\hbar}. \tag{57}$$

It is straightforward to calculate the commutation relations among the creation and annihilation operators in the momentum space:

$$\begin{aligned}
[a(\vec{p}), a^\dagger(\vec{q})] &= \frac{1}{L^3} \int d\vec{x} d\vec{y} [\psi(\vec{x}) e^{-i\vec{p}\cdot\vec{x}/\hbar}, \psi^\dagger(\vec{y}) e^{i\vec{q}\cdot\vec{y}/\hbar}] \\
&= \frac{1}{L^3} \int d\vec{x} d\vec{y} \delta(\vec{x} - \vec{y}) e^{-i\vec{p}\cdot\vec{x}/\hbar} e^{i\vec{q}\cdot\vec{y}/\hbar} \\
&= \frac{1}{L^3} \int d\vec{x} e^{-i(\vec{p}-\vec{q})\cdot\vec{x}/\hbar} \\
&= \delta_{\vec{p},\vec{q}}.
\end{aligned} \tag{58}$$

This is nothing but the commutation relation for harmonic oscillators. Obviously,

$$[a(\vec{p}), a(\vec{q})] = [a^\dagger(\vec{p}), a^\dagger(\vec{q})] = 0. \tag{59}$$

It is instructive to rewrite the Hamiltonian in the momentum space. The free part of the Hamiltonian is

$$\begin{aligned}
H_0 &= \int d\vec{x} \psi^* \frac{-\hbar^2 \Delta}{2m} \psi \\
&= \int d\vec{x} \frac{1}{L^3} \sum_{\vec{p}} \sum_{\vec{q}} a^\dagger(\vec{p}) e^{-i\vec{p}\cdot\vec{x}/\hbar} \frac{-\hbar^2 \Delta}{2m} a(\vec{q}) e^{i\vec{q}\cdot\vec{x}/\hbar} \\
&= \int d\vec{x} \frac{1}{L^3} \sum_{\vec{p}} \sum_{\vec{q}} a^\dagger(\vec{p}) e^{-i\vec{p}\cdot\vec{x}/\hbar} \frac{\vec{q}^2}{2m} a(\vec{q}) e^{i\vec{q}\cdot\vec{x}/\hbar} \\
&= \frac{1}{L^3} \sum_{\vec{p}} \sum_{\vec{q}} a^\dagger(\vec{p}) \frac{\vec{q}^2}{2m} a(\vec{q}) L^3 \delta_{\vec{p},\vec{q}} \\
&= \sum_{\vec{p}} \frac{\vec{p}^2}{2m} a^\dagger(\vec{p}) a(\vec{p}).
\end{aligned} \tag{60}$$

The free Hamltonian simply countes the number of particles in a given momentum state $a^\dagger(\vec{p})a(\vec{p})$ and assigns the energy $\vec{p}^2/2m$ accordingly. The interaction Hamltonian is somewhat more complicated

$$
\begin{aligned}
\Delta H &= \int d\vec{x} d\vec{y} \frac{1}{2} \psi^*(\vec{x})\psi^*(\vec{y}) V(\vec{x}-\vec{y})\psi(\vec{y})\psi(\vec{x}) \\
&= \frac{1}{2L^6} \sum_{\vec{p},\vec{p}',\vec{q},\vec{q}'} \int d\vec{x} d\vec{y} a^\dagger(\vec{p}) a^\dagger(\vec{p}') V(\vec{x}-\vec{y}) a(\vec{q}') a(\vec{q}) e^{-i(\vec{p}-\vec{q})\cdot\vec{x}/\hbar} e^{-i(\vec{p}'-\vec{q}')\cdot\vec{y}/\hbar} \\
&= \frac{1}{2L^3} \sum_{\vec{p},\vec{p}',\vec{q},\vec{q}'} \int d\vec{x} a^\dagger(\vec{p}) a^\dagger(\vec{p}') V(\vec{x}-\vec{y}) a(\vec{q}') a(\vec{q}) \delta_{\vec{p}+\vec{p}',\vec{q}+\vec{q}'} e^{-i(\vec{p}-\vec{q})\cdot\vec{x}/\hbar} \\
&= \frac{1}{2} \sum_{\vec{p},\vec{p}',\vec{q},\vec{q}'} V(\vec{p}-\vec{q}) a^\dagger(\vec{p}) a^\dagger(\vec{p}') a(\vec{q}') a(\vec{q}) \delta_{\vec{p}+\vec{p}',\vec{q}+\vec{q}'}, \qquad (61)
\end{aligned}
$$

with

$$V(\vec{p}-\vec{q}) = \frac{1}{L^3} \int d\vec{x} V(\vec{x}) e^{-i(\vec{p}-\vec{q})\cdot\vec{x}/\hbar}. \qquad (62)$$

Kronecker's delta represents the momentum conservation in the scattering process due to the potential V.

Therefore the interpretation of the Hamiltonian is quite simple. The free part counts the number of particles and associates the kinetic energy $\vec{p}^2/2m$ for each of them according to its momentum. The potential term causes scattering, by annihilating two particles in momentum states $\vec{q}, \vec{q}'$ and create them in different momentum states $\vec{p}, \vec{q}'$ with the amplitude $V(\vec{p}-\vec{q})$ (note that $\vec{p}-\vec{q} = \vec{q}' - \vec{q}'$ because of the momentum conservation).

At this point, it is useful to note that one can introduce a term in the potential that can change the number of particles, such as $a^\dagger a^\dagger a^\dagger aa$ for $2 \to 3$ body scattering if there is need for it. Indeed, when we discuss quantization of radiation field (namely, theory of photons by quantizating classical Maxwell field), we see a term in the Hamiltonian which creates or annihilates a photon. Such an interaction can never be described in conventional Schrödinger wave functions, but is possible in quantum field theory.

4.8 Background Potential

The Hamiltonian Eq. (42) describes interacting bosons but we are often interested in a system in a background potential. A good example is the electrons in an atom, where all of them are moving in the background Coulomb potential due to the nucleus. In this case, the correct field-theory Hamiltonian is

$$H = \int d\vec{x}\psi^* \left(\frac{-\hbar^2 \Delta}{2m} - \frac{Ze^2}{|\vec{x}|} \right) \psi + \int d\vec{x} d\vec{y} \frac{1}{2} \psi^*(\vec{x}) \psi^*(\vec{y}) \frac{e^2}{|\vec{x} - \vec{y}|} \psi(\vec{y}) \psi(\vec{x}). \tag{63}$$

where the second term in the parantheses is the Coulomb pontential due to the nucleus, while the last term is the Coulomb repulsion among electrons. In this case, a more convenient expansion of the field operator would be

$$\psi(\vec{x}) = \sum_{nlm} a_{nlm} u_{nlm}(\vec{x}), \tag{64}$$

where a_{nlm} is the annihilation operator and the c-number $u_{nlm}(\vec{x})$ is the complete basis for expanding the field operator with. Then the state with certain states filled can be written down as

$$a^\dagger_{1s} a^\dagger_{2p,m=1} |0\rangle \qquad \text{etc.} \tag{65}$$

But this Hamiltonian gives bosons instead of fermions. How to obtain fermions out of quantized Schrödinger field is the issue in the next section.

5 Fermions

We have seen that the quantized Schrödinger field gives multi-body states of identical bosons. But we also need fermions to describe electrons, protons, etc. How do we do that?

The trick is to go back to the commutation relations Eq. (22). Instead of them, we can use *anti-commutation* relations

$$\{\psi(\vec{x}), \psi^\dagger(\vec{y})\} = \delta(\vec{x} - \vec{y}), \qquad \{\psi, \psi\} = \{\psi^\dagger, \psi^\dagger\} = 0. \tag{66}$$

The notation is $\{A, B\} = AB + BA$ instead of $[A, B] = AB - BA$. This small change flips the statistics completely and the same Hamiltonian Eq. (42) describes a system of identical fermions.

One noteworthy point is that $\psi(\vec{x})^{\dagger 2} = \frac{1}{2}\{\psi(\vec{x})^\dagger, \psi(\vec{x})^\dagger\} = 0$. What this means is that one cannot create two particles at the same position, an expression of Pauli's exclusion principle for fermions.

Here are a few useful identities. Similarly to the identity of commutators $[A, BC] = [A, B]C + B[A, C]$, we find

$$\begin{aligned}
[A, BC] &= ABC - BCA \\
&= ABC + BAC - BAC - BCA \\
&= \{A, B\}C - B\{A, C\}
\end{aligned} \tag{67}$$

Similarly,

$$\begin{aligned}
[AB, C] &= ABC - CAB \\
&= ABC + ACB - ACB - CAB \\
&= A\{B, C\} - \{A, C\}B.
\end{aligned} \tag{68}$$

Again it is useful to calculate the commutator $[H, \psi^\dagger(\vec{x})]$ for later purposes.

$$\begin{aligned}
&[H, \psi^\dagger(\vec{x})] \\
&= [\int d\vec{y} \left(\psi^\dagger(\vec{y}) \frac{-\hbar^2 \Delta_{\vec{y}}}{2m} \psi(\vec{y}) + \int d\vec{z} \frac{1}{2} \psi^\dagger(\vec{y}) \psi^\dagger(\vec{z}) V(\vec{y} - \vec{z}) \psi(\vec{z}) \psi(\vec{y}) \right), \psi^\dagger(\vec{x})] \\
&= \int d\vec{y} \psi^\dagger(\vec{y}) \frac{-\hbar^2 \Delta_{\vec{y}}}{2m} \{\psi(\vec{y}), \psi^\dagger(\vec{x})\} \\
&\quad + \int d\vec{y} d\vec{z} \frac{1}{2} \psi^\dagger(\vec{y}) \psi^\dagger(\vec{z}) V(\vec{y} - \vec{z}) [\psi(\vec{z}) \psi(\vec{y}), \psi^\dagger(\vec{x})] \\
&= \frac{-\hbar^2 \Delta_{\vec{x}}}{2m} \psi^\dagger(\vec{x}) + \int d\vec{z} \psi^\dagger(\vec{x}) \psi^\dagger(\vec{z}) V(\vec{x} - \vec{z}) \psi(\vec{z}).
\end{aligned} \tag{69}$$

Consider a two-particle state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \int d\vec{x}_1 d\vec{x}_2 \Psi(\vec{x}_1, \vec{x}_2) \psi^\dagger(\vec{x}_1) \psi^\dagger(\vec{x}_2) |0\rangle. \tag{70}$$

Because $\{\psi^\dagger(\vec{x}_1), \psi^\dagger(\vec{x}_2)\} = 0$, or more explicitly

$$\psi^\dagger(\vec{x}_1) \psi^\dagger(\vec{x}_2) = -\psi^\dagger(\vec{x}_2) \psi^\dagger(\vec{x}_1), \tag{71}$$

the c-number function Ψ is hence anti-symmetric under the exchange of two positions

$$\Psi(\vec{x}_1, \vec{x}_2) = -\Psi(\vec{x}_2, \vec{x}_1). \tag{72}$$

Such a state indeed describes identical fermions.

All other aspects of the discussions remain the same as in the case of bosons. A general k-body state is

$$|\Psi\rangle = \int d\vec{x}_1 \cdots d\vec{x}_n \frac{1}{\sqrt{n!}} \Psi(\vec{x}_1, \cdots, \vec{x}_n) \psi^\dagger(\vec{x}_1) \cdots \psi^\dagger(\vec{x}_n)|0\rangle \tag{73}$$

with the anti-symmetry of the Schrödinger wave function $\Psi(\vec{x}_1, \cdots, \vec{x}_n)$ required because of the anti-commutation relation $\psi^\dagger(\vec{x}_i)\psi^\dagger(\vec{x}_j) = -\psi^\dagger(\vec{x}_j)\psi^\dagger(\vec{x}_i)$. The number operator is $N = \int d\vec{x}\psi^\dagger(\vec{x})\psi(\vec{x})$.

One weird point about fermion is that the classical limit of the field $\phi = \hbar^{1/2}\psi$ satisfies the anti-commutation relation

$$\{\phi(\vec{x}), \phi^\dagger(\vec{y})\} = \hbar\delta(\vec{x} - \vec{y}) \to 0 \tag{74}$$

in the classical limit. This is certainly not an ordinary function or number. It is called a Grassmann number. The classical limit of Fermi field therefore does not have a direct physical meaning, even though we need to deal with Grassmann number in path integrals for Fermi fields.