Quantum field theory and Green’s function

- Condensed matter physics studies systems with large numbers of identical particles (e.g. electrons, phonons, photons) at finite temperature.
- Quantum field theory arises naturally if we consider a quantum system composed by a large number of identical particles at finite or zero temperature.

1.1. Quantum statistical physics

1.1.1. Classical statistical physics

Classical statistical physics tells us that in the grand canonical ensemble, the expectation value of a thermal dynamic quantity, which will be called $X$ here, can be written as:

$$
\langle X \rangle = \frac{\sum_n X_n \exp[-\beta (E_n - \mu N_n)]}{\sum_n \exp[-\beta (E_n - \mu N_n)]}
$$

(1.1)

where $\beta = 1/T$ (here the Boltzmann constant $k_B$ is set to unity) and $\mu$ is the chemical potential. Here, we sum over all possible states of the system ($\sum_n$). For the $n$th state, the total energy of the whole system is $E_n$; the particle number is $N_n$ and the value of the quantity $X$ is $X_n$.

1.1.2. Quantum statistical physics

For a quantum system (at finite temperature $T$), we can rewrite this formula in terms of quantum operators

$$
\langle X \rangle = \sum_n \langle n | \hat{X} \exp[-\beta (\hat{H} - \mu \hat{N})] | n \rangle = \frac{\text{Tr} [\hat{X} \exp[-\beta (\hat{H} - \mu \hat{N})]]}{\text{Tr} [\exp[-\beta (\hat{H} - \mu \hat{N})]]}
$$

(1.2)

where $\sum_n$ sums over a complete orthonormal basis of the Hilbert space $| n \rangle$. $\hat{H}$ is the Hamiltonian, $\hat{N}$ is the particle number operator and $\hat{X}$ is the quantum operator of the quantity that we want to compute. The sum $\sum_n \langle n | \ldots | n \rangle$ is also known as a trace $\text{Tr}$. It is easy to verify that the above formula for $\langle X \rangle$ is independent of the choice of basis.

Here, we will not prove this operator formula, because it is not part of the main focus of this lecture. Instead, we will only demonstrate that by choosing a proper basis, this (quantum) operator formula recovers the classical formula shown above, and therefore, the operator formula is a natural quantum generalization of classical statistical physics.

If $[\hat{H}, \hat{N}] = 0$, we can choose the common eigenstates of $\hat{H}$ and $\hat{N}$ as our basis. In this basis, we have

$$
\hat{H} | n \rangle = E_n | n \rangle
$$

(1.3)

and

$$
\hat{N} | n \rangle = N_n | n \rangle
$$

(1.4)

where $E_n$ is the eigen-energy and $N_n$ is the eigen-value of the particle number operator.

Using this basis, it is easy to check that

$$
\exp[-\beta (\hat{H} - \mu \hat{N})] | n \rangle = \exp[-\beta (E_n - \mu N_n)] | n \rangle
$$

(1.5)

and therefore,
\begin{equation}
\langle X \rangle = \frac{\sum (\langle n | \hat{X} \exp[-\beta(\hat{H} - \mu \hat{N})] | n \rangle)}{\sum (\langle n | \exp[-\beta(\hat{H} - \mu \hat{N})] | n \rangle)} = \frac{\sum_{a} \langle n | \hat{X} | n \rangle \exp[-\beta(\mu N_a)]}{\sum_{a} \langle n | \exp[-\beta(\mu N_a)]} = \frac{\sum_{a} X_a \exp[-\beta(\mu N_a)]}{\sum_{a} \exp[-\beta(\mu N_a)]}
\end{equation}

Here, we define \( X_a = \langle n | \hat{X} | n \rangle \).

Note: the quantum field theory used in particle physics is the \( T \to 0 \) limit of this finite temperature theory.

Q: What happens if \( [\hat{H}, \hat{N}] \neq 0 \)?

A: If \( [\hat{H}, \hat{N}] \neq 0 \), it implies that in this system, the particle number is not conserved. As will be discussed in later chapters, particle conservation law is related with the U(1) phase symmetry for charge neutral particles (or the U(1) gauge symmetry for charged particles). The absences of particle conservation implies the breaking of phase/gauge symmetry, which means that the system is a superfluid/superconductor.

### 1.2. Second quantization

- The terminology of “second quantization” is due to historical reasons. We are NOT quantizing something for a second time. We are just using a new basis to handle indistinguishable particles.

Q: Why do we want to use second quantization?

A: It is the most convenient way to handle a large number of indistinguishable particles.

#### 1.2.1. Wavefunctions for distinguishable particles

It is easy to write down quantum wavefunctions for systems composed by distinguishable particles. For example, if we have two distinguishable particles, particle one in state \( \psi_1 \) and particle two in \( \psi_2 \), the wavefunction is

\[ \Psi(r_1, r_2) = \psi_1(r_1) \psi_2(r_2) \]  

If we have \( n \) distinguishable particles, the wavefunction can be written as

\[ \Psi(r_1, r_2, r_3, ..., r_n) = \psi_1(r_1) \psi_2(r_2) ... \psi_n(r_n) \]  

Here, the \( i \)th particle is in the quantum state \( \psi_i \) for \( i = 1, 2, ... n \).

#### 1.2.2. Wave functions for indistinguishable particles

For indistinguishable particles, the wavefunction is very complicated, if the particle number is large. This is because we need to ensure that the wavefunction is symmetric (anti-symmetric) for bosons (fermions). If we have two indistinguishable particles, one particle in the state \( \psi_1 \) and the other in the state \( \psi_2 \), the wavefunction is

\[ \Psi(r_1, r_2) = \psi_1(r_1) \psi_2(r_2) \pm \psi_2(r_1) \psi_1(r_2) \]  

Here, the + sign is for bosons and the - sign is for fermions. It is easy to check that the wavefunction is symmetric or anti-symmetric

\[ \Psi(r_1, r_2) = \pm \Psi(r_2, r_1) \]  

If we have 3 indistinguishable particles, the wavefunction contains \( 3! = 6 \) terms

\[ \Psi(r_1, r_2, r_3) = \psi_1(r_1) \psi_2(r_2) \psi_3(r_3) \pm \psi_1(r_1) \psi_3(r_2) \psi_2(r_3) \pm \psi_2(r_1) \psi_1(r_2) \psi_3(r_3) \pm \psi_2(r_1) \psi_3(r_2) \psi_1(r_3) \pm \psi_3(r_1) \psi_1(r_2) \psi_2(r_3) \pm \psi_3(r_1) \psi_2(r_2) \psi_1(r_3) \]  

If we have \( n \) indistinguishable particles,

\[ \Psi(r_1, r_2, r_3, ..., r_n) = \sum_{\mathcal{P}} (\pm 1)^{\mathcal{P}} \psi_{\mathcal{P}}(r_1) \psi_{\mathcal{P}}(r_2) ... \psi_{\mathcal{P}}(r_n) \]  

where \( \mathcal{P} \) represents all permutations. For a system with \( n \) particles, there are \( n! \) different permutations and thus the r.h.s. has \( n! \) terms. For a system with a large number of indistinguishable particles, it is an extremely complicated to write down its wavefunction in this way. For example, for a system with just ten particles, \( n=10 \), there are \( 10! \approx 2.6 \) million terms, which is impossible to write down. In condensed matter physics, a typical system has huge number of particles (~\( 10^{23} \)) and thus we need a better way to write down our quantum theory.
Note: in particle physics, although one typically studies systems with a very small number of particles (e.g. two particles collides with each other in a collider), however, it is still necessary to consider large numbers of particles because we have “virtue particles”. For example, the E&M interactions between two electrons is realized by exchanging virtual photons. If one takes into account these virtual particles, the particle number is not very small, and thus we shall use second quantization.

1.2.3. Fock space

The reason why it is hard to write down wavefunctions for indistinguishable particles is because when we write do the wavefunction, we need to specify which particle is in which quantum state. For example, $\psi_j(r_j)$ means the particle number $j$ is in the quantum state $\psi_j$. This procedure is natural for distinguishable particles, where we do know that particle $i$ is in a certain quantum state. However, for indistinguishable particles, we don’t actually know which particle is in this state, because we cannot distinguish the particles. In other words, the traditional way to write down a wavefunction is designed for distinguishable particles. For indistinguishable particles, we need to first treat them as distinguishable particles, and then repeat the wavefunction using all different permutations to make the wavefunction symmetric/anti-symmetric. This procedure is not natural and is very complicated.

For indistinguishable particles, it is more natural to use the occupation number basis, which is known as the Fock space. In the Fock space, a many-body quantum state is written in terms of occupation numbers:

$$|\Psi\rangle = |n_1, n_2, n_3 \ldots nN\rangle$$

(1.13)

where $n_i$ is the number of particles in state $|\psi_i\rangle$ ($n_i$ is known as the occupation number). Here we don’t specify which particle is in the state $|\psi_i\rangle$. Instead, we just count the number of particles in this state. In this approach, the particle are indistinguishable automatically and thus all the complicates mentioned above are avoided.

1.2.4. Creation and annihilation operators:

In the Fock space, all physical operators can be written in terms of creation and annihilation operators. The creation operator increases the occupation number by 1 and the annihilation operator reduces the occupation number by 1.

For bosons, we have

$$b_i^+ |n_1, n_2, n_3 \ldots nN\rangle = \sqrt{n_i + 1} |n_1, n_2, \ldots n_i + 1, \ldots nN\rangle$$

(1.14)

$$b_i |n_1, n_2, n_3 \ldots nN\rangle = \sqrt{n_i} |n_1, n_2, \ldots n_i - 1, \ldots nN\rangle$$

(1.15)

and it is easy to check that these operators obey the following commutation relations:

$$[b_i, b_j] = [b_i^+, b_j^+] = 0$$

(1.16)

$$[b_i, b_j^+] = \delta_{ij}$$

(1.17)

For fermions, due to the Pauli exclusive principle, each quantum state can at most have one particle (so $n_i = 0$ or 1).

$$c_i^+ |\ldots, 1, \ldots\rangle = 0$$

(1.18)

$$c_i^+ |\ldots, 0, \ldots\rangle = (-1)^{\sum c_i^+} |\ldots, 1, \ldots\rangle$$

(1.19)

$$c_i |\ldots, 1, \ldots\rangle = 0$$

(1.20)

$$c_i^+ |\ldots, 0, \ldots\rangle = (-1)^{\sum c_i} |\ldots, 0, \ldots\rangle$$

(1.21)

It is easy to check that fermion creation/annihilation operators obey anti-commutation relations:

$$\{c_i, c_j\} = [c_i^+, c_j^+] = 0$$

(1.22)

$$\{c_i, c_j^+\} = \delta_{ij}$$

(1.23)

Note: the factor $(-1)^{\sum c_i^+} n$ is dropped in many textbooks, because $|\psi\rangle$ and $-|\psi\rangle$ represent the same quantum state. However, this factor is curial to ensure the anti-commutation relation $\{c_i, c_j^+\} = \delta_{ij}$. We will study this factor later when we examine 1D quantum systems.

1.2.5. Particle number operator

For bosons, using the definition above, it is easy to check that

$$b_i^+ b_j |\ldots, n_i, \ldots\rangle = n_i |\ldots, n_i, \ldots\rangle$$

(1.24)
So the eigenvalues of the operator $b_i^+ b_i$ is the number of particles in quantum state $i$, which is known as the occupation number. In other words, the particle number quantum operator for bosons in the quantum state $|\psi_i\rangle$ is
\begin{equation}
\hat{n}_i = b_i^+ b_i
\end{equation}
(1.25)

The total particle number operator is
\begin{equation}
\hat{N} = \sum_i \hat{n}_i = \sum_i b_i^+ b_i
\end{equation}
(1.26)

For fermions, it is easy to notice that
\begin{align}
&\quad \quad \quad \quad c_i^+ c_i \quad \text{for all } \quad \text{is zero} \\
&c_i^+ c_i [\ldots \ldots \text{total}] = 0
\end{align}
(1.27)

\begin{align}
&\quad \quad \quad \quad c_i^+ c_i \quad \text{for all } \quad \text{is one} \\
&c_i^+ c_i [\ldots \ldots \text{total}] = 1
\end{align}
(1.28)

Therefore, the particle number operator for fermions in the quantum state $|\psi_i\rangle$ is
\begin{equation}
\hat{n}_i = c_i^+ c_i
\end{equation}
(1.29)

As a result, the total particle number operator is
\begin{equation}
\hat{N} = \sum_i \hat{n}_i = \sum_i c_i^+ c_i
\end{equation}
(1.30)

In the next a couple of sections, we will only consider fermions as our example ($c$ and $c^+$), but the same conclusions are applicable for bosons ($b$ and $b^+$)

### 1.2.6. Quantum states

In the Fock space, all quantum states can be written in terms of creation and annihilation operators. First, we need to define the vacuum (ground states in high energy physics) $|0\rangle$ by assuming that there is one and only one state in the Fock space that is annihilated by any annihilation operators. This state is our vacuum
\begin{equation}
c_i |0\rangle = 0 \quad \text{for any } c_i
\end{equation}
(1.31)

It is easy to check that this quantum states has zero particle
\begin{equation}
\hat{N} |0\rangle = \sum_i c_i^+ c_i |0\rangle = 0
\end{equation}
(1.32)

Then, for an arbitrary states with one particle (a one-particle state), we can write it as
\begin{equation}
|\psi\rangle = \sum_i a_i c_i^+ |0\rangle
\end{equation}
(1.33)

where $a_i$ is any complex numbers.

For two particle states, they can be written as
\begin{equation}
|\psi\rangle = \sum_{i_1, i_2} a_{i_1} a_{i_2} c_{i_1}^+ c_{i_2}^+ |0\rangle
\end{equation}
(1.34)

For $n$ particle states, they can be written as
\begin{equation}
|\psi\rangle = \sum_{i_1, \ldots, i_n} a_{i_1} a_{i_2} \ldots a_{i_n} c_{i_1}^+ c_{i_2}^+ \ldots c_{i_n}^+ |0\rangle
\end{equation}
(1.35)

### 1.2.7. quantum operators

Any quantum operator can be written in terms of creation and annihilation operators $c$ and $c^+$:
\begin{equation}
X = \sum_{i, j, k \ldots} c_{i_1} c_{i_2} \ldots c_{i_n} c_{j_1} c_{j_2} \ldots c_{j_m} c_{k_1} c_{k_2} \ldots c_{k_p}
\end{equation}
(1.36)

If every term in this operator has $m$ annihilation operators and $m'$ creation operators, this operator is known as a $(m + m')$ fermion operator.

### 1.2.8. Physical observables and correlation functions

Since all quantum operators can be written in terms of creation and annihilation operators, the expectation value of any physical observable can be written in terms of the expectation values of creation and annihilation operators:
\begin{equation}
\langle X \rangle = \langle c_{i_1} c_{i_2} \ldots c_{i_n} c_{j_1} c_{j_2} \ldots c_{j_m} c_{k_1} c_{k_2} \ldots c_{k_p} \rangle
\end{equation}
(1.37)

Therefore, in second quantization, anything we need to compute reduces to objects like this: $c_{i_1} c_{i_2} \ldots c_{i_n} c_{j_1} c_{j_2} \ldots c_{j_m} c_{k_1} c_{k_2} \ldots c_{k_p}$. This type of objects are known as correlation functions. If there are $N$ creation and annihilation operators, it is known as a $N$-point correlation function.
Here, $N = m + m'$. 

Q: What are the simplest nontrivial correlation functions? Here, “simplest” means that we want the number of creation and annihilation operator to be as small as possible. “nontrivial” means the correlation function need to be nonzero.

A: If the particle number is conserved ($\{\hat{H}, \hat{N}\} = 0$, which is true for most of the cases we study), they are the two-point correlation functions. This is because, if $[\hat{H}, \hat{N}] = 0$, we can prove that $\langle c_{k1} c_{k2} \ldots c_{km} c_{q1}^\dagger c_{q2}^\dagger \ldots c_{qm}^\dagger \rangle = 0$ if $m \neq m'$. In other words, if we want to have a nontrivial correlation function, it must have the same number of creation and annihilation operators. Therefore, we only need to consider $N$-point correlation functions when $N$ is even. The smallest positive even integer is 2, so the simplest nontrivial correlation functions are two-point correlation functions $\langle c_k c_{k'} \rangle$. The next one is four-point correlation $\langle c_{k1} c_{k2} c_{q1}^\dagger c_{q2}^\dagger \rangle$.

Proof: As shown above, if $[\hat{H}, \hat{N}] = 0$, we know that particle number is a conserved quantity and thus we can choose the common eigenstates of $\hat{H}$ and $\hat{N}$ as our basis. In this basis, we have

$$\langle c_{k_1} c_{k_2} \ldots c_{k_m} c_{q_1}^\dagger c_{q_2}^\dagger \ldots c_{q_m}^\dagger | n \rangle = \sum_n \left( \langle n | c_{k_1} c_{k_2} \ldots c_{k_m} c_{q_1}^\dagger c_{q_2}^\dagger \ldots c_{q_m}^\dagger | n \rangle \right) \frac{\exp(-\beta(E_n - \mu N_n))}{\sum_n \exp(-\beta(E_n - \mu N_n))}$$

(1.38)

Because $|n\rangle$ is the eigenstate of the total particle number operator $\hat{N}$, we know that the quantum state $|n\rangle$ has $N_n$ particles. Define

$$|\psi\rangle = c_{k_1} c_{k_2} \ldots c_{k_m} c_{q_1}^\dagger c_{q_2}^\dagger \ldots c_{q_m}^\dagger |n\rangle$$

(1.39)

because a creation operator increase the particle number by 1, while an annihilation operator reduce it by 1, it is easy to note that $|\psi\rangle$ has $N_n + m - m'$ particles.

If $m' \neq m$, $N_n + m' - m \neq N_n$, which means that the quantum states $|n\rangle$ and $|\psi\rangle$ has different number of particles, i.e. they are both eigen states of $\hat{N}$, but they have different eigenvalues. In quantum mechanics, we learned that two eigenstates of the same operator are orthogonal, if they have different eigenvalues, so we know immediately that $\langle n | \psi \rangle = 0$. And therefore, $\langle n | c_{k_1} c_{k_2} \ldots c_{k_m} c_{q_1}^\dagger c_{q_2}^\dagger \ldots c_{q_m}^\dagger | n \rangle = 0$. As a result, the correlation function $\langle c_{k_1} c_{k_2} \ldots c_{k_m} c_{q_1}^\dagger c_{q_2}^\dagger \ldots c_{q_m}^\dagger \rangle = 0$.

Note: If $[\hat{H}, \hat{N}] = 0$, we will have nonzero correlation functions with $m \neq m'$. For example, in superfluids, $\langle b \rangle \neq 0$, and in superconductors $\langle c_b c_b \rangle = 0$. These cases will be considered later.

1.2.9. Summary

- The terminology of “second quantization” is due to historical reasons. We are NOT quantizing something for a second time. We are just using a new basis to handle indistinguishable particles.
- In both high energy and condensed matter physics, quantum field theory utilize the “second quantization” construction. The reason is because quantum field theory deals with more than one indistinguishable palaces, and the second quantization formulas are the most natural way to describe this type of physics.
- In second quantization (same is true for quantum field theory), any physical quantities are reduced to computing various correlation functions.
- If particle number is conserved, only correlation functions with same number of creation and annihilation operators are nontrivial.
- The order matters: $\langle c_k c_{k'} \rangle \neq \langle c_{k'} c_k \rangle$. Therefore, depending on the way to order the creation/annihilation operators, we can define different correlation functions. This topics will be address in the next section.

1.3. Hamiltonian in second quantization

Let’s consider a Hamiltonian with three terms: the kinetic energy $H_K$, the potential energy $H_P$ and interactions between different particles $H_I$, 

$$H = H_K + H_P + H_I$$

(1.40)

1.3.1. Potential energy

For particles in a potential $U(\vec{r})$, the total potential energy (summed over all particles) is

$$P.E. = \int d\vec{r} U(\vec{r}) \rho(\vec{r})$$

(1.41)

where $\rho(\vec{r})$ is the particle density at $\vec{r}$. In second quantization, particle density is

$$\rho(\vec{r}) = \psi^*(\vec{r}) \psi(\vec{r})$$

(1.42)

Here, $\psi^*(\vec{r})$ creates an electron at $\vec{r}$ and $\psi(\vec{r})$ annihilate an electron at $\vec{r}$. Therefore, the potential energy part of the Hamiltonian is