221B Lecture Notes
Quantum Field Theory II (Fermi Systems)

1 Statistical Mechanics of Fermions

1.1 Partition Function

In the case of fermions, we had learnt that the field operator satisfies the anti-commutation relation and becomes Grassmann-odd number in the classical limit. Clearly, a Grassmann-odd classical Fermi field is not an observable as no measurement would yield a Grassmann-odd number as a result. However, this issue is not completely academic because the path integral requires the classical integration variable: we need to integrate over Grassmann-odd Fermi field $\psi(\vec{x}, t)$.

What is the definition of an integral over a Grassmann-odd number? I do not go into details, but rather give you a consistent definition for our use: the integration is *the same* as the differentiation! To make it explicit what I mean, let me take one Grassmann-odd number ψ (no $\vec{x}$, t dependence). Any function of ψ can always be expanded as

$$f(\psi) = f(0) + f'(0)\psi \tag{1}$$

because the Taylor expansion vanishes at higher orders in ψ due to its Grassmann-odd nature $\psi^2 = \frac{1}{2}\{\psi, \psi\} = 0$. The definition of the Grassmann integral is

$$\int d\psi f(\psi) = f'(0). \tag{2}$$

One could have tried to take $f(0)$ instead as the definition of the integral rather than $f'(0)$; however, it would violate the shift invariance of the integration variable $\psi \to \psi' = \psi + \eta$. We would like to retain this property to be analogous to the bosonic integral which satisfies $\int_{-\infty}^{\infty} dx f(x) = \int_{-\infty}^{\infty} dx f(x+a)$. To see this, let us imagine defining the integral to pick up the piece $f(0)$ instead of $f'(0)$. Then $\int d\psi f(\psi) = f(0)$ by definition. However, $\int d\psi f(\psi+\eta)$ for a constant η would be $\int d\psi f(\psi+\eta) = \int d\psi (f(0) + (\psi+\eta)f'(0))$. Since this (wrong) definition would pick all ψ independent pieces, the result would be $f(0) + \eta f'(0)$, which is different from the result without the shift. On the other hand, picking up the piece proportional to ψ yields $f'(0)$ in both cases.

The partition function is given by the same expression as the bosonic case

$$Z = \int \mathcal{D}\psi(\vec{x},\tau)\mathcal{D}\psi^\dagger(\vec{x},\tau) \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \int d\vec{x} \left(\psi^* \hbar\dot{\psi} + \psi^* \frac{-\hbar^2\Delta}{2m}\psi\right)\right]. \tag{3}$$

However, there is another peculiarity with Fermi field: we need to take the anti-periodic boundary condition $\psi(\hbar\beta) = -\psi(0)$ instead of the periodic boundary condition. This can be shown by carefully working out the trace $\mathrm{Tr} e^{-\beta H}$ in terms of fermionic path integral (see the appendix). We do not go into the detail of the derivation here, but proceed with the anti-periodic boundary condition. Fourier expansion is then modified

$$\psi(\vec{x},\tau) = \frac{1}{L^{3/2}} \sum_{\vec{p},n} z_{\vec{p},n} e^{i\vec{p}\cdot\vec{x}/\hbar} e^{\pi i(2n-1)\tau/\hbar\beta}. \tag{4}$$

The partition function is

$$\begin{aligned} Z &= \prod_{\vec{p},n} \int dz^*_{\vec{p},n} dz_{\vec{p},n} e^{-(\pi i(2n-1)+\beta(\vec{p}^2/2m-\mu)) z^*_{\vec{p},n} z_{\vec{p},n}} \\ &= \prod_{\vec{p},n} \left[\pi i(2n-1) + \beta\left(\frac{\vec{p}^2}{2m} - \mu\right)\right], \end{aligned} \tag{5}$$

where we used the rule for the Grassmann integrals after Taylor expanding the exponential up to order $z^*_{\vec{p},n} z_{\vec{p},n}$ for each $\vec{p}$, n. This time we use the formula

$$\prod_{n=1}^{\infty} \left(1 + \frac{x^2}{(2n-1)^2}\right) = \cosh\frac{\pi x}{2}, \tag{6}$$

and find

$$Z = c \prod_{\vec{p}} \cosh\frac{\beta}{2}\left(\frac{\vec{p}^2}{2m} - \mu\right) = c \prod_{\vec{p}} \left(e^{\beta(\vec{p}^2/2m-\mu)} + 1\right) e^{-\beta(\vec{p}^2/2m-\mu)/2}. \tag{7}$$

The energy expectation value is hence

$$\langle E \rangle = -\frac{\partial}{\partial\beta} \ln Z \bigg|_{\beta\mu} = \sum_{\vec{p}} \frac{\vec{p}^2}{2m}\left[-\frac{1}{2} + \frac{1}{e^{\beta(\vec{p}^2/2m-\mu)} + 1}\right], \tag{8}$$

which must be familiar to you except the zero-point energy contribution. It is interesting to note that the zero-point energy is negative for fermions.[1]

[1] If you have both bosons and fermions with the same mass, the zero-point enegies precisely cancel. This is the idea behind supersymmetry.

1.2 Fermi Liquid

At zero temperature, the fermions fill up energy levels up to the Fermi level $\mu = \varepsilon_F$. This is the degenerate Fermi gas. Many Fermi systems can be approximated by Fermi gas even when they are interacting. Such systems are called Fermi liquids. Electrons in the conduction band of a metal are to a good approximation a degenerate Fermi gas already at room temperature. Other examples are electrons in white dwarfs, neutrons in neutron stars, and to some extent, protons and neutrons in nuclei. We have discussed many of these already. The discussions here will be brief.

For a free Fermi gas, the Hamiltonian including the chemical potential is

$$H = \sum_{\vec{p}} \left(\frac{p^2}{2m} - \mu \right) b(\vec{p})^\dagger b(\vec{p}). \tag{9}$$

Similarly to the case of bosons, the energy becomes negative for $\vec{p}^2/2m \leq \mu$, but unlike bosons, it does not imply the development of a condensate. The point is that you can create a negative-energy particle to reduce the energy, but you can do so only once for each mode in a Fermi system, while you can keep decreasing energy by puttingin macroscopic number of particles until the interaction stops it in a Bose system. Therefore, there is a stable ground state even in the absence of interactions

$$|g\rangle = \prod_{\vec{p}, \vec{p}^2/2m > \mu} |0\rangle \prod_{\vec{p}, \vec{p}^2/2m < \mu} b(\vec{p})^\dagger |0\rangle \tag{10}$$

with the Hamiltonian eigenvalue

$$E_g = \sum_{\vec{p}, \vec{p}^2/2m < \mu} \left(\frac{\vec{p}^2}{2m} - \mu \right) < 0. \tag{11}$$

It is useful to introduce the concept of a “hole.” If you remove a particle from the above ground state, it actually *increases* the energy. A useful way to see this is to introduce a new set of creation/annihilation operators by

$$c(\vec{p}) = b(-\vec{p})^\dagger, \qquad c(\vec{p})^\dagger = b(-\vec{p}). \tag{12}$$

Note that the anti-commutation relation remains the same $\{c(\vec{p}), c(\vec{p})^\dagger\} = \{b(-\vec{p})^\dagger, b(-\vec{p})\} = 1$. The ground state above is annihilated by the new annihilation operator $c(\vec{p})|g\rangle = b(-\vec{p})^\dagger|g\rangle = 0$. The Hamiltonian can also be rewritten as

$$H = \sum_{\vec{p},\vec{p}^2/2m>\mu} \left(\frac{p^2}{2m} - \mu\right) b(\vec{p})^\dagger b(\vec{p}) + \sum_{\vec{p},\vec{p}^2/2m<\mu} \left(\mu - \frac{p^2}{2m}\right) c(\vec{p})^\dagger c(\vec{p}) + E_0. \quad (13)$$

Now both $b^\dagger$ and $c^\dagger$ creation operators have positive energies and allow the standard particle interpretation. An important point, however, is that the "hole" created by the creation operator $c^\dagger$ carries a positive electric charge. The momentum of the hole is the opposite of the momentum you have removed: that is why we chose $c(\vec{p})^\dagger = b(-\vec{p})$ instead of $b(\vec{p})$. The concept of hole is very useful in band structure in condensed matter systems, atomic levels, nuclear levels, and as we will see later, relativistic Dirac equation.

What about interactions among fermions? It is interesting to note that the delta-function interaction in the action

$$-\int d\vec{x}\frac{\lambda}{2}\psi^*\psi^*\psi\psi \quad (14)$$

identically vanishes because it involves product of ψ at the same position in space $\psi(\vec{x})\psi(\vec{x}) = 0$. It is a simple consequence of Pauli's exclusion principle that two fermions cannot occupy the same position. This simple fact already suggests that certain effects of interactions identically vanish for Fermi systems as opposed to Bose systems. However, because of the spin degrees of freedom, we must introduce two separate fields $\psi_\uparrow$ and $\psi_\downarrow$ to represent spin up and down states, and the interaction

$$-\int d\vec{x}\frac{\lambda}{2}\psi_\uparrow^*\psi_\downarrow^*\psi_\downarrow\psi_\uparrow \quad (15)$$

is possible. Of course, a general potential term in the action

$$-\frac{1}{2}\int d\vec{x}d\vec{y}V(\vec{x}-\vec{y})\psi^*(\vec{y})\psi^*(\vec{x})\psi(\vec{x})\psi(\vec{y}) \quad (16)$$

does not identically vanish. If the potential V has a typical order of magnitude V_0, and if you consider the Fermi level ε_F much higher than V_0, the interactions deep in the degenerate Fermi gas reshuffle states among themselves, and do not change the Slater determinant, as we discussed before. The only effects appear close to the Fermi surface $\varepsilon_F - V_0 \lesssim E \lesssim \varepsilon_F + V_0$.

1.3 Condensation of Fermion Pairs

When the interaction is attractive between fermions, it can cause a condensate, somewhat analogous to the bosons, but the condensate can happen only for fermion *pairs* because a “classical anti-commuting” condensate does not make any sense. Let me briefly discuss how a pair-wise condensate can occur in Fermi systems.

What you do is very similar to what you did with bosons in non-zero momentum modes. Starting with the Hamiltonian of the type

$$\begin{aligned} H = & \sum_{\vec{p}} \left(\frac{\vec{p}^2}{2m} - \mu \right) a^\dagger(\vec{p}) a(\vec{p}) \\ & - \sum_{\vec{p}} V(\vec{p}, \vec{p}_2, \vec{p}_3, \vec{p}_4) a^\dagger(\vec{p}_1) a^\dagger(\vec{p}_2) a(\vec{p}_3) a(\vec{p}_4) \delta_{\vec{p}_1+\vec{p}_2, \vec{p}_3+\vec{p}_4}. \end{aligned} \tag{17}$$

We consider the variational state

$$\prod_{\vec{p}}{}' [\alpha_{\vec{p}} + \beta_{\vec{p}} a^\dagger(\vec{p}) a^\dagger(-\vec{p})] |0\rangle \tag{18}$$

with $|\alpha_{\vec{p}}|^2 + |\beta_{\vec{p}}|^2 = 1$. Here and below, the notation $\prod_{\vec{p}}{}'$ takes the product only over a half of the momentum modes to avoid double counting of $\vec{p}$ and $-\vec{p}$. Taking

$$\alpha_{\vec{p}} = 0, \quad \beta_{\vec{p}} = 1 \qquad \text{for } \frac{\vec{p}^2}{2m} < \mu, \tag{19}$$

$$\alpha_{\vec{p}} = 1, \quad \beta_{\vec{p}} = 0 \qquad \text{for } \frac{\vec{p}^2}{2m} > \mu, \tag{20}$$

corresponds to the conventional “vacuum”

$$\prod_{|\vec{p}| < p_F} a^\dagger(\vec{p}) |0\rangle. \tag{21}$$

But depending on the nature of the potential, the state with both $\alpha_{\vec{p}}, \beta_{\vec{p}} \neq 0$ may give you a lower energy expectation value. If this is the case, there is a condensate

$$\langle a(\vec{p}) a(-\vec{p}) \rangle = \alpha_{\vec{p}} \beta_{\vec{p}} \neq 0. \tag{22}$$

This type of variational state is called Bardeen–Cooper–Schrieffer (BCS) state. It is used in the superfluidity of ^{3}He ($S = 1$, $L = 1$), the superconductivity ($S = 0$, $L = 0$; the original application), high-T_c superconductor

($S = 0$, $L = 2$), and neutron stars. The case of superconductivity of course has the electromagnetic interaction as important gredients and we will come back to this in later lecture notes. In any case, $\alpha_{\vec{p}} \to 1$ well above the Fermi surface and $\beta_{\vec{p}} \to 1$ well below the Fermi surface, while both of them are non-vanishing close to the Fermi surface. In other words, Fermi surface is "fuzzy," not as sharp as in standard Fermi liquid.

Bogoliubov transformation needed to diagonalize the Hamiltonian for fermions is similar to that for bosons but slightly different. We would like to preserve the anti-commutation relation $\{a(\vec{p}), a^\dagger(\vec{q})\} = \delta_{\vec{p},\vec{q}}$. Therefore, we can define a new creation/annihilation operators by

$$b(\vec{p}) = a(\vec{p}) \cos\eta_{\vec{p}} + a^\dagger(-\vec{p}) \sin\eta_{\vec{p}}. \tag{23}$$

It is easy to check that $\{b(\vec{p}), b^\dagger(\vec{q})\} = \delta_{\vec{p},\vec{q}}$, and hence they quality as creation/annhilation operators. The unitarity operator that relates two sets of operators is

$$U = \prod_{\vec{p}}{}' e^{-\eta_{\vec{p}}(a(\vec{p})a(-\vec{p}) - a^\dagger(-\vec{p})a^\dagger(\vec{p}))}, \qquad U a(\vec{p}) U^\dagger = b(\vec{p}). \tag{24}$$

The ground state with a condensate is annihilated by $b(\vec{p})$

$$0 = b(\vec{p})|gs\rangle = U a(\vec{p}) U^\dagger |gs\rangle. \tag{25}$$

The solution to this equation is simply

$$U^\dagger |gs\rangle = |0\rangle. \tag{26}$$

Unlike in the case of bosons, we can expand the exponential explicitly and find

$$|gs\rangle = U|0\rangle = \prod_{\vec{p}}{}' (\cos\eta_{\vec{p}} + a^\dagger(-\vec{p}) a^\dagger(\vec{p}) \sin\eta_{\vec{p}})|0\rangle. \tag{27}$$

This is indeed the BCS state. Excitations above the BCS state are given by acting $b^\dagger(\vec{p})$ on the ground state, and they are fermions.

A Anti-periodic Boundary Condition

Here is the derivation why fermion fields must satisfy the anti-periodic boundary condition. It turns out it is a somewhat long story.

Let us start with a Lagrangian

$$L = \psi^* i\hbar\dot{\psi} - \hbar\omega\psi^*\psi. \tag{28}$$

$\psi(t)$ depends only on time but not on space. The "classical" Euler–Lagrange equation is

$$i\hbar\dot{\psi} - \omega\psi = 0, \tag{29}$$

with an obvious solution

$$\psi(t) = \psi(0)e^{-i\omega t}. \tag{30}$$

To see what this Lagrangian describes quantum mechanically, note that the ψ can be regarded as the canonical coordinate, while its canonically conjugate momentum is $\partial L/\partial\dot{\psi} = i\dot{\psi}$. Therefore, we find the canonical anti-commutation relation

$$\{\psi, \psi^*\} = 1. \tag{31}$$

This defines a two-dimensional Hilbert space spanned by

$$|0\rangle, \qquad |1\rangle = \psi^*|0\rangle, \tag{32}$$

where the state $|0\rangle$ is defined by the requirement $\psi|0\rangle = 0$. The Hamiltonian of the system is

$$H = \hbar\omega\left(\psi^*\psi - \frac{1}{2}\right). \tag{33}$$

(The zero-point energy was added to be consistent with the result from the path integral.) In other words, this is a two-state system with energies $\pm\frac{1}{2}\hbar\omega$.

Now we need to find the decomposition of unity analogous to $\int |x\rangle dx\langle x| = 1$ to be used to derive the path integral for ψ. Note that the conventional path integral was derived using the position eigenstates $x|q\rangle = q|q\rangle$. Likewise, we need the eigenstates of the operator ψ. It can be obtained in analogy to coherent states

$$\psi|\eta\rangle = \eta|\eta\rangle, \tag{34}$$

where the coherent state $|\eta\rangle$ is defined by

$$|\eta\rangle = |0\rangle - \eta|1\rangle. \tag{35}$$

Note that η is a Grassman number, and anti-commutes with the annihilation operator ψ even though it is not an operator. That guarantees that

$$\psi|\eta\rangle = \psi|0\rangle - \psi\eta|1\rangle = \eta\psi|1\rangle = \eta|0\rangle = \eta|\eta\rangle, \tag{36}$$

where we used $\eta^2 = \{\eta, \eta\}/2 = 0$ at the very last step. This coherent state, however, is not normalized, because

$$\langle \eta | \eta \rangle = 1 + \eta^* \eta = e^{\eta^* \eta}, \tag{37}$$

where the last expression is more convenient for later purposes. Now it is easy to see that the following decomposition of unity holds:

$$1 = \int d\eta^* d\eta |\eta\rangle e^{-\eta^* \eta} \langle \eta|. \tag{38}$$

Starting from the r.h.s., we can check that

$$\begin{aligned} \int d\eta^* d\eta |\eta\rangle e^{-\eta^*\eta} \langle \eta| &= \int d\eta^* d\eta (|0\rangle - \eta|1\rangle) e^{-\eta^*\eta} (\langle 0| - \eta^* \langle 1|) \\ &= \int d\eta^* d\eta \left(-\eta^*\eta |0\rangle\langle 0| + \eta\eta^* |1\rangle\langle 1|\right) \\ &= |0\rangle\langle 0| + |1\rangle\langle 1|. \end{aligned} \tag{39}$$

Here and below, we stick to the convention that the integrals are done from right to left, so that $\int d\eta d\eta^* \eta^* \eta = \int d\eta \eta = 1$.

We need another quantity, $\langle \eta' | e^{-iHt/\hbar} | \eta \rangle$, analogous to $\langle x' | e^{-iH\Delta t/\hbar} | x \rangle = (2\pi m / i\Delta t)^{1/2} e^{i(m(x'-x)^2/\Delta t - V(x)\Delta t)/\hbar}$ for small t for the ordinary path integral. This can be calculated easily

$$\langle \eta' | e^{-iH\Delta t/\hbar} | \eta \rangle = \langle \eta' | e^{-i\omega\psi^*\psi\Delta t} | \eta \rangle = \langle \eta' | e^{-i\omega\eta'^*\eta\Delta t} | \eta \rangle = e^{-i\omega\eta'^*\eta\Delta t} e^{\eta'^*\eta}. \tag{40}$$

for small Δt.

Now we can keep inserting the decomosition of unity between the initial and the final states.

$$\begin{aligned} &\langle \eta(t) | e^{-iHt/\hbar} | \eta(0) \rangle \\ &= \lim_{N\to\infty} \int \langle \eta_N | e^{-iH\Delta t/\hbar} | \eta_{N-1} \rangle e^{-\eta^*_{N-1}\eta_{N-1}} d\eta^*_{N-1} d\eta_{N-1} \langle \eta_{N-1} | e^{-iH\Delta t/\hbar} | \eta_{N-2} \rangle \\ &\quad e^{-\eta^*_{N-2}\eta_{N-2}} d\eta^*_{N-2} d\eta_{N-2} \cdots e^{-\eta^*_1\eta_1} d\eta^*_1 d\eta_1 \langle \eta_1 | e^{-iH\Delta t/\hbar} | \eta_0 \rangle \\ &= \lim_{N\to\infty} \int e^{-i\omega\eta^*_N\eta_{N-1}} e^{\eta^*_N\eta_{N-1}} e^{-\eta^*_{N-1}\eta_{N-1}} d\eta^*_{N-1} d\eta_{N-1} e^{-i\omega\eta^*_{N-1}\eta_{N-2}} e^{\eta^*_{N-1}\eta_{N-2}} \\ &\quad e^{-\eta^*_{N-2}\eta_{N-2}} d\eta^*_{N-2} d\eta_{N-2} \cdots e^{-\eta^*_1\eta_1} d\eta^*_1 d\eta_1 e^{-i\omega\eta^*_1\eta_0} e^{\eta^*_1\eta_0} \\ &= \int d\eta^*(t) d\eta(t) \exp\left[\frac{i}{\hbar} \int dt (\eta^* i\hbar\dot{\eta} - \hbar\omega\eta^*\eta)\right]. \end{aligned} \tag{41}$$

Note that $\eta^*(t) = \eta_N^*$ and $\eta(0) = \eta_0$ are not integrated over. This defines the path integral.

Now comes the question of the trace. The trace of an operator $\mathcal{O}$ is defined by

$$\mathrm{Tr}\mathcal{O} = \langle 0|\mathcal{O}|0\rangle + \langle 1|\mathcal{O}|1\rangle. \tag{42}$$

The point is to rewrite it in terms of an η integral. It is easy to show that

$$\begin{aligned}\int d\eta^* d\eta \langle \eta|\mathcal{O}|\eta\rangle e^{-\eta^*\eta} &= \int d\eta^* d\eta (\langle 0| - \eta^*\langle 1|)\mathcal{O}(|0\rangle - \eta|1\rangle)e^{-\eta^*\eta} \\ &= \int d\eta^* d\eta(-\eta^*\eta\langle 0|\mathcal{O}|0\rangle + \eta^*\eta\langle 1|\mathcal{O}|1\rangle) \\ &= \langle 0|\mathcal{O}|0\rangle - \langle 1|\mathcal{O}|1\rangle. \end{aligned}\tag{43}$$

This is off by a sign for the second term for the trace we wanted to calculate. We can avoid this if we had taken not $\langle\eta|$ but rather $\langle -\eta|$:

$$\int d\eta^* d\eta \langle -\eta|\mathcal{O}|\eta\rangle e^{-\eta^*\eta} = \langle 0|\mathcal{O}|0\rangle + \langle 1|\mathcal{O}|1\rangle. \tag{44}$$

This is the origin of the anti-periodic boundary condition.

We finally calculate $\langle \eta_N|e^{-\beta H}|\eta_0\rangle$ in terms of a path integral, and to obtain the trace from this result, we do the following integral

$$Z = \int d\eta^*(t) d\eta(t) \exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau(\eta^*(-i\hbar)\dot{\eta} + \hbar\omega\eta^*\eta)\right] \tag{45}$$

with the understanding that $\eta(t)$, $\eta^*(t)$ follow the anti-periodic boundary conditions.