Tutorial 1

Path integral formulation and the Hubbard-Stratonovich transformation

References: Altland & Simons Chapter 4 & 6.

Introduction

In this tutorial we have two objectives: (i) *Imaginary time coherent state path integral formalism* - to prove the identity (4). The motivation will be to show that quantum averages of many-body systems in thermal equilibrium can be computed using functional integrals over field configurations. (ii) *The Hubbard-Stratonovich transformation* - To provide a rigorous formalism in which the phenomenological Ginzburg-Landau (GL) theory can be related to an underlying microscopic theory theory.

Coherent state path integrals

When we study single-body problems, the particle can be described by its position operator $\mathbf{q}$. To get the path integral we then work in an eigen basis of this operator and calculate the propagator $\langle \mathbf{q}'t'|\mathbf{q},t\rangle$, for example, which turns out to be related to integration over the paths $\mathbf{q}(t)$.

In field theory we have a field, i.e., a “position” operator at each point in space $\phi(x)$. We anticipate that the path integral will be related to an integration over the field configurations $\phi(x,t)$. To make sense of this, it is clear that we first need to work in a basis that diagonalizes the field operators. The states that do this are called coherent states.

To be more specific, a coherent state is an eigenstate of an annihilation operator a

$$|\psi\rangle = e^{\zeta\psi a^\dagger}|0\rangle$$

where $\zeta = 1$ ($\zeta = -1$) for Bosons (Fermions), such that $a|\psi\rangle = \psi|\psi\rangle$. Remember that our field operators are annihilation operators labeled by the spatial coordinates, so these are clearly the type of states we need in order to construct the path integral.

If we have many annihilation operators labeled by some index i (which in our case will be the spatial coordinate), we write a simultaneous eigenstate as

$$|\psi\rangle = e^{\zeta\psi_i a_i^\dagger}|0\rangle\,,$$

such that $a_i |\psi\rangle = \psi_i |\psi\rangle$.

There are some crucial differences between the states corresponding to boson fields and those corresponding to fermion fields. Below we list the important properties of the two cases.

Bosonic coherent states

In the simpler case a describes a bosonic degree of freedom and ψ is simply a c-number. We will make use of three basic identities: first the overlap between two coherent states

$$\langle \psi_1 | \psi_2 \rangle = e^{\bar{\psi}_1 \psi_2}. \tag{1}$$

The second is the resolution of identity which follows directly from (1)

$$1 = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} |\psi\rangle \langle\psi| \tag{2}$$

Here we use the notation that ψ is a vector with a discrete set of components ψ_i corresponding to the underlying Fock space. When studying a field theory in the continuum limit, this will be $\psi(x)$. In the general case the above notations mean $\bar{\psi}\psi \equiv \sum_i \bar{\psi}_i \psi_i$ and $d\bar{\psi} d\psi \equiv \prod_i \frac{d\bar{\psi}_i d\psi_i}{\pi}$. Finally, the third identity is the Gaussian integral of the complex variables ψ and $\bar{\psi}$

$$\int d\bar{\psi} d\psi e^{-\bar{\psi} A \psi} = \frac{1}{|A|}$$

where A is a matrix with a positive definite Hermitian part.

Fermionic coherent states

If the operator a describes a fermionic field things become a bit more complicated. To see this, let us assume again that $|\psi\rangle$ is an eigen state such that $a_i |\psi\rangle = \psi_i |\psi\rangle$. The only way to make this consistent with the anti-commutation relations between different a's is to demand that different $\psi's$ anti-commute as well. We therefore need special numbers that anti-commute. These are known as Grassmann numbers, and they satisfy:

$$\psi_i \psi_j = -\psi_j \psi_i.$$

The operation of integration and differentiation with these numbers are defined as follows

$$\int d\psi = 0; \int d\psi \psi = 1$$

and $\partial_\psi \psi = 1$.

The overlap between two coherent states and the resolution of identity remain in the form of (1) and (2). The Gaussian integral on the other hand is significantly different

$$\int d\bar{\psi} d\psi e^{-\bar{\psi} A \psi} = |A| \tag{3}$$

where A can be any matrix.

Derivation of the path integral

In what follows we will prove the central identity

$$Z = \mathrm{Tr} e^{-\beta(\hat{H}-\mu\hat{N})} = \int D[\psi,\bar{\psi}] e^{-\int_0^\beta d\tau \left(\bar{\psi}\partial\tau\psi + H[\bar{\psi},\psi] - \mu N[\bar{\psi},\psi]\right)}. \tag{4}$$

where H and N are the Hamiltonian and particle number respectively and $\psi, \bar{\psi}$ are c-numbers (Grassmann numbers) in the case that the particles have Bosonic (Fermionic) mutual statistics, assigned to each point of space and "time" τ. The boundary conditions of this path integral is $\psi(0) = \zeta\psi(\beta)$ and $\bar{\psi}(0) = \zeta\bar{\psi}(\beta)$.

As mentioned above, our motivation will be computing expectation values of quantum many-body systems in thermal equilibrium. For example, if we have an operator $A[a, a^\dagger]$, its expectation value will be

$$\langle \hat{A} \rangle = \frac{1}{Z} \int D[\psi,\bar{\psi}] A[\psi,\bar{\psi}] e^{-\int_0^\beta d\tau \left(\bar{\psi}\partial\tau\psi + H[\bar{\psi},\psi] - \mu N[\bar{\psi},\psi]\right)}.$$

Let start with the definition of the trace

$$Z = \mathrm{Tr} e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_n \langle n | e^{-\beta(\hat{H}-\mu\hat{N})} | n \rangle \tag{5}$$

Notice that each term in this sum is the probability amplitude of finding the the system at the same Fock state it started in, i.e. $|n\rangle$, after a time $t = i\hbar\beta$, which, as you know, can be written as a Feynman path integral. In the first step we will want to get rid of the summation over n. To do so we insert the resolution of identity (2) into equation (5)

$$Z = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \sum_n \langle n|\psi\rangle \langle \psi | e^{-\beta(\hat{H}-\mu\hat{N})} | n \rangle$$

We can sum over n using the resolution of identity $1 = \sum_n |n\rangle\langle n|$ but we first need to commute $\langle n|\psi\rangle$ with $\langle \psi | e^{-\beta(\hat{H}-\mu\hat{N})} | n \rangle$. In the case of bosonic particles this is just a number and it commutes with anything. In the case of fermions Grassmann numbers are involved and we need to be more careful. If we expand the matrix elements in terms of the Grassmann variables, we find an additional sign:

$$Z = \int d\bar{\psi} d\psi e^{-\bar{\psi}\psi} \langle \zeta\psi | e^{-\beta(\hat{H}-\mu\hat{N})} | \psi \rangle \tag{6}$$

Now let us continue to the second step: we divide the imaginary-time evolution operator into M small steps

$$e^{-\beta(\hat{H}-\mu\hat{N})} = \left(e^{-\delta(\hat{H}-\mu\hat{N})}\right)^M$$

where $\delta = \beta/M$. In the third step we insert M resolutions of identity in the expectation value in equation (6)

$$\langle \zeta\psi | [e^{-\delta\left(\hat{H}-\mu\hat{N}\right)}]^M | \psi \rangle = \int \prod_{m=1}^{M} d\bar{\psi}^m d\psi^m e^{-\sum_m \bar{\psi}^m \psi^m} \times \tag{7}$$
$$\langle \zeta\psi | \psi^M \rangle \langle \psi^M | e^{-\delta\left(\hat{H}-\mu\hat{N}\right)} | \psi^{M-1} \rangle \cdots \langle \psi^2 | e^{-\delta\left(\hat{H}-\mu\hat{N}\right)} | \psi^1 \rangle \langle \psi^1 | e^{-\delta\left(\hat{H}-\mu\hat{N}\right)} | \psi \rangle$$

Expanding in small δ, we have

$$\begin{aligned}
\langle \psi^{m+1} | e^{-\delta\left(\hat{H}-\mu\hat{N}\right)} | \psi^m \rangle &\approx \langle \psi^{m+1} | 1 - \delta\left(\hat{H} - \mu\hat{N}\right) | \psi^m \rangle \\
&= \langle \psi^{m+1} | \psi^m \rangle \left(1 - \delta\left(H[\bar{\psi}^{m+1}, \psi^m] - \mu N[\bar{\psi}^{m+1}, \psi^m]\right)\right) \\
&\approx e^{\bar{\psi}^{m+1}\psi^m - \delta\left(H[\bar{\psi}^{m+1},\psi^m] - \mu N[\bar{\psi}^{m+1},\psi^m]\right)},
\end{aligned}$$

where we have defined $H[\bar{\psi}^{m+1}, \psi^m] = \frac{\langle \psi^{m+1} | \hat{H} | \psi^m \rangle}{\langle \psi^{m+1} | \psi^m \rangle}$.

Now if we insert this expression in (6) we get

$$Z = \int \prod_{m=0}^{M} d\bar{\psi}^m d\psi^m e^{-\delta \sum_{m=0}^{M}\left[\left(\frac{\bar{\psi}^m - \bar{\psi}^{m+1}}{\delta}\right)\psi^m + H[\bar{\psi}^{m+1},\psi^m] - \mu N[\bar{\psi}^{m+1},\psi^m]\right]}$$

with $\psi^0 = \zeta\psi^{M+1} = \psi$. Finally, in the fourth step we take $M \to \infty$ and obtain

$$Z = \int D[\psi, \bar{\psi}] e^{-\int_0^\beta d\tau \left(\bar{\psi}\partial\tau\psi + H[\bar{\psi},\psi] - \mu N[\bar{\psi},\psi]\right)}$$

where

$$D[\bar{\psi}, \psi] \equiv \lim_{M\to\infty} \prod_{m=0}^{M} d\bar{\psi}^m d\psi^m$$

The integration is to be carried over fields satisfying $\psi(\beta) = \zeta\psi(0)$. It is very important to note that by neglecting the time derivative term we resume to the classical integration over configurations of the fields ψ and $\bar{\psi}$. Indeed the time derivative term takes into account the effects of the non-trivial (anti-) commutation between a_i and $a_i^\dagger$ which have now been transferred to fields ψ_i and $\bar{\psi}_i$ which always have trivial (anti-) commutation relations.

To be more specific, we usually discuss an interacting Hamiltonian of the form

$$S = \int_0^\beta d\tau \left[\sum_{ij} \bar{\psi}_i \left[(\partial_\tau - \mu)\,\delta_{ij} + h_{ij} \right] \psi_j + \sum_{ijkl} V_{ijkl} \bar{\psi}_i(\tau)\bar{\psi}_j(\tau)\psi_k(\tau)\psi_l(\tau) \right]$$

To compute path integrals we usually transform to the Fourier basis where the derivative operators are diagonal. This procedure applies also for the imaginary time

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_\nu \psi(\nu) e^{-i\nu\tau}$$

in which case the action takes the form

$$S = \sum_{n,ij} \bar{\psi}_{in} \left[(-i\nu_n - \mu)\,\delta_{ij} + h_{ij} \right] \psi_{jn} +$$

$$+ \frac{1}{\beta} \sum_{ijkl,n_i} V_{ijkl} \bar{\psi}_{in_1} \bar{\psi}_{jn_2} \psi_{kn_3} \psi_{ln_4} \delta_{n_1+n_2,n_3+n_4}.$$

To obey the boundary conditions $\psi(0) = \zeta\psi(\beta)$ we choose the following frequencies in the wave functions $e^{-i\nu\tau}$

$$\nu_n = \begin{cases} \frac{2n\pi}{\beta} & \text{Bosons} \\ \frac{(2n+1)\pi}{\beta} & \text{Fermion} \end{cases}$$

These imaginary-time frequencies are known as *Matsubara frequencies*. Summing over them is a whole story to itself. You will see an example in the exercise. I want to note that in the limit of zero temperature ($\beta \to \infty$) the sum becomes a simple integral $\frac{1}{\beta}\sum_{\nu_n} \to \int_{-\infty}^{\infty} \frac{d\nu}{2\pi}$.

The Hubbard-Stratonovich transformation

In this tutorial we will learn a general method to relate a Ginzburg-Landau theory to the underlying microscopic theory. For example let us consider the GL theory of a ferromagnet

$$F_{GL} = \int d^3x \left[-\alpha \mathbf{m} \nabla^2 \mathbf{m} + a m^2 + \beta m^4 \right].$$

Here, if $a < 0$ a transition to a ferromagnetic state may occur.

To see how to relate this theory to an underlying microscopic theory let us consider an interacting model of fermions

$$Z = \int D[\bar{\psi}, \psi] e^{-S}$$

$$S = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s + u \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right] \tag{8}$$

Notice that the local interactions may be reorganized in the following manner

$$\bar{\psi}_\uparrow(x) \bar{\psi}_\downarrow(x) \psi_\downarrow(x) \psi_\uparrow(x) = -\frac{2}{3} \mathbf{s}(x) \cdot \mathbf{s}(x)$$

where $\mathbf{s}(x) = \frac{1}{2} \bar{\psi}_s \sigma_{ss'} \psi_{s'}$ and thus the action is equivalently given by

$$S = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s - g \mathbf{s} \cdot \mathbf{s} \right], \tag{9}$$

where $g = \frac{2}{3} u$.

Now we will employ the Hubbard-Stratonovich transformation which relies on the following identity

$$\int D[\mathbf{m}] \exp \left[- \int_0^\beta d\tau d^3x \left(m^2 - 2\mathbf{m} \cdot \mathbf{s} \right) \right] \tag{10}$$

$$= \underbrace{\int D[\mathbf{m}] \exp \left[- \int_0^\beta d\tau d^3x \left(\mathbf{m} - \mathbf{s} \right)^2 \right]}_{N} \exp \left[\int_0^\beta d\tau d^3x s^2 \right] \tag{11}$$

$$= N \exp \left[\int_0^\beta d\tau d^3x s^2 \right], \tag{12}$$

where N does not depend on the field $\mathbf{s}$. Thus, equation (8) may be equivalently written as follows

$$Z = \frac{1}{N} \int D[\bar{\psi}, \psi, \mathbf{m}] e^{-S_{HS}} \tag{13}$$

where

$$S_{HS} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s - 2g \mathbf{m} \cdot \mathbf{s} + g m^2 \right]$$

Notice that the action above resembles a mean-field decoupling of the interaction term. To see this substitute $\mathbf{s} = \mathbf{M} + \delta\mathbf{s}$ in the interaction term, where $\mathbf{M}$ is the mean-field, and neglect terms of order $O(\delta s^2)$

$$\mathbf{s}\cdot\mathbf{s} = (\mathbf{M} + \delta\mathbf{s})(\mathbf{M} + \delta\mathbf{s}) \approx 2\mathbf{M}\cdot\mathbf{s} - M^2$$

However, there is a crucial difference: $\mathbf{M}$ is a mean-field with a single value whereas the field $\mathbf{m}$ fluctuates and we integrate over all possible paths of this field. Actually, equation (13) is exact, we made no approximations in deriving it. As you will see in the exercise the saddle point approximation of this theory gives the self-consistent mean-field approximation obtained from a variational method. This observation suggests that the field $\mathbf{m}$, introduced by some formal manipulations, may be interpreted as a local magnetization field.

Finally, let us discuss how we can use the HS theory (13) to obtain an effective theory for the magnetization field $\mathbf{m}$. The standard way is to integrate over the Fermions. Since the $\mathbf{m}$-field interacts with the fermions, their integration will generate terms containing the $\mathbf{m}$ field. First let us rewrite the theory as follows

$$S_{HS} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\underbrace{\left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\delta_{ss'}}_{G^{-1}} - \underbrace{g\mathbf{m}\cdot\sigma_{ss'}}_{X}\right)\psi_{s'} + gm^2\right]$$

Formally, the fermionic part of the path integral has the quadratic form

$$\int d\bar{\psi}d\psi\, e^{-\bar{\psi}A\psi},$$

where $A = G^{-1} - X[\mathbf{m}]$. Thus using (3) we can perform the integral over the fermions which gives

$$Z = \frac{1}{N}\int D[\mathbf{m}]|A|\, e^{-gm^2} = \frac{1}{N}\int D[\mathbf{m}]\, e^{-gm^2+\log|A|} = \frac{1}{N}\int D[\mathbf{m}]\, e^{-gm^2+\mathrm{Tr}\log A}$$

The trace of the logarithm can be expanded perturbatively in small X in the following manner:

$$\mathrm{Tr}\ \log A = \mathrm{Tr}\log\left(G^{-1} - X\right) = \mathrm{Tr}\ \log G^{-1} + \mathrm{Tr}\log\left(1 - GX\right) =$$

$$\mathrm{Tr}\ \log G^{-1} + \mathrm{Tr}\ \left[-GX + \frac{1}{2}GXGX + ...\right]$$

Now since X is linear in m each order gives the corresponding order in the Ginzburg-Landau theory. The first order vanishes, as can be anticipated on symmetry grounds. The second order term, if expanded in momentum basis, gives the quadratic term

$$\frac{1}{2}\mathrm{Tr}\left[GXGX\right] = \frac{g^2}{\beta\Omega}\sum_{\mathbf{q},\omega} \mathit{\Pi}\left(\mathbf{q},\omega\right)\mathbf{m}_{\mathbf{q}}(\omega)\mathbf{m}_{-\mathbf{q}}(-\omega),$$

where

$$\Pi = \frac{1}{\beta\Omega}\sum_{\mathbf{k}\nu}\frac{1}{-i\nu+\frac{k^2}{2m}-\mu}\cdot\frac{1}{-i(\nu+\omega)+\frac{(\mathbf{k}+\mathbf{q})^2}{2m}-\mu},$$

and we have used the fact that G is diagonal in spin space and that the Pauli matrices are traceless. We can expand this in small $\mathbf{q}$ and get the parameters of the Ginzburg-Landau theory:

$$a = g - \mathit{\Pi}(0,0),$$

and

$$\alpha = \frac{1}{2}\left(\frac{\partial^2\Pi(\mathbf{q},0)}{\partial q^2}\right)\bigg|_{q=0}.$$

Of course β will be derived from a higher order term with four powers of X.