

Concepts in Condensed Matter Physics:

Tutorial II

Coherent State Path Integrals and the Hubbard-Stratonovich Transformation

References: Chapter 4 & 6 of “Condensed Matter Field Theory” by Altland & Simons.

1 Introduction

In this tutorial we have two objectives: (i) *Derive the imaginary-time coherent state path integral formalism* - namely, to prove the central identity in Eq.(9). 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) *Introduce the Hubbard-Stratonovich transformation* - providing a rigorous formalism in which the phenomenological Ginzburg-Landau (GL) theory can be related to an underlying microscopic theory.

2 Coherent state path integrals

When we study single-body problems, the particle can be described by its position operator \vec{q} . To get the path integral we then work in an eigenbasis of this operator and calculate the propagator $\langle \vec{q}_i, t_i | \vec{q}_f, t_f \rangle$, for example, which turns out to be related to integration over the paths $\vec{q}(t)$ from \vec{q}_i at t_i to \vec{q}_f at t_f .

In field theory we have a field displacement operator at each point in space $\hat{\phi}(x)$. We anticipate that the field theory path integral will be related to an integration over all field configurations $\hat{\phi}(x, t)$. To make sense of this, it is clear that we first need to work in a basis that diagonalizes the field operators: $\hat{\phi}(x) | \phi(x) \rangle = \phi(x) | \phi(x) \rangle$.

In Condensed Matter theory, many models are formulated in terms of creation and annihilation operators: a_i^\dagger and a_i (or $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$ in the continuum). Therefore, in order to write a field theory for these cases we need to work in a different eigenbasis, namely, that of the annihilation operators.

2.1 Coherent states

Coherent states are eigenstates of the annihilation operator, a , and are given by

$$|\psi\rangle = \exp[\zeta\psi a^\dagger] |0\rangle, \quad (1)$$

where $\zeta = 1$ ($\zeta = -1$) for bosons (fermions), and $|0\rangle$ is the vacuum satisfying $a|0\rangle = 0$. It is easy to check that $a|\psi\rangle = \psi|\psi\rangle$. 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

$$|\psi\rangle = \exp\left[\zeta \sum_i \psi_i a_i^\dagger\right] |0\rangle, \quad (2)$$

such that $a_i|\psi\rangle = \psi_i|\psi\rangle$ for all i . Importantly, these states are overcomplete and can thus be used to span the Fock space. 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.

2.1.1 Bosonic coherent states

In the simpler case a_i are bosonic operators and ψ_i are simply c-numbers. We will make use of three basic identities:

1. The overlap of two coherent states:

$$\langle\psi_1|\psi_2\rangle = e^{\bar{\psi}_1\psi_2}. \quad (3)$$

2. The identity operator can be resolved in terms of coherent states as:

$$\mathbb{I} = \int d\bar{\psi}d\psi e^{-\bar{\psi}\psi} |\psi\rangle \langle\psi|. \quad (4)$$

This follows directly from the overlap. Here we use the notation that ψ is a vector with a discrete set of components ψ_i corresponding to the underlying Fock space. Therefore, in the above expression we mean that $\bar{\psi}\psi \equiv \sum_i \bar{\psi}_i\psi_i$, and $d\bar{\psi}d\psi \equiv \prod_i \frac{d\bar{\psi}_i d\psi_i}{\pi}$.

3. The Gaussian integral of the complex variables ψ and $\bar{\psi}$:

$$\int d\bar{\psi}d\psi e^{-\bar{\psi}A\psi} = \frac{1}{\det(A)} \quad (5)$$

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

2.1.2 Fermionic coherent states

If the operators a_i are fermionic things become a bit more complicated. To see this, let us assume again that $|\psi\rangle$ is an eigenstate of a_i such that $a_i a_j |\psi\rangle = \psi_i \psi_j |\psi\rangle$. But since $a_i a_j = -a_j a_i$ the only way to keep things consistent is to demand that different ψ 's (the eigenvalues) anticommute as well. These anticommuting numbers are called Grassmann numbers (or variables), and they are defined to satisfy:

$$\psi_i \psi_j = -\psi_j \psi_i . \quad (6)$$

They are also defined to follow special integration and differentiation rules (in order to reproduce the correct path integral for fermions):

$$\int d\psi_i = 0 , \quad (7a)$$

$$\int d\psi_i \psi_i = 1 , \quad (7b)$$

$$\partial_{\psi_i} \psi_j = \delta_{i,j} . \quad (7c)$$

These are defined such that the overlap between two coherent states and the resolution of identity remain unchanged, i.e., as in Eq.(3) and Eq.(4) (up to the $1/\pi$ factors). The Gaussian integral on the other hand is significantly different and reads:

$$\int d\bar{\psi} d\psi e^{-\bar{\psi} A \psi} = \det(A) , \quad (8)$$

where A can be any matrix.

2.2 Derivation of the coherent state path integral

In what follows we will prove the following central identity

$$\mathcal{Z} = \text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-\int_0^\beta d\tau [\bar{\psi} \partial_\tau \psi + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi)]} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-\mathcal{S}[\bar{\psi}, \psi]} , \quad (9)$$

where \mathcal{Z} is the partition function, H and N are the Hamiltonian and particle number operators respectively, and ψ and $\bar{\psi}$ are c-numbers (or Grassmann numbers) assigned to each point of space, i or x , and imaginary time, τ . The boundary conditions of this path integral are:

$$\psi(0) = \zeta\psi(\beta) , \quad (10)$$

and the corresponding expression for $\bar{\psi}$. As mentioned above, our motivation is computing expectation values of quantum many-body systems in thermal equilibrium. For example, if we have an operator $A(\psi, \psi^\dagger)$, its expectation value will be given by

$$\langle A(a^\dagger, a) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\bar{\psi}, \psi] A(\bar{\psi}, \psi) e^{-\int_0^\beta d\tau [\bar{\psi} \partial \tau \psi + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi)]} . \quad (11)$$

We start with the definition of the trace as a sum over the diagonal matrix elements in some base:

$$\mathcal{Z} = \text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})} = \sum_n \langle n | e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle , \quad (12)$$

where $|n\rangle$ is a complete set of Fock states¹. The first step is to get rid of the summation over $|n\rangle$. To do so we insert the resolution of identity, as given in Eq.(4), into Eq.(12) and manipulate to get:

$$\begin{aligned} \mathcal{Z} &= \int d\bar{\psi}_0 d\psi_0 e^{-\bar{\psi}_0 \psi_0} \sum_n \langle n | \psi_0 \rangle \langle \psi_0 | e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle \\ &= \int d\bar{\psi}_0 d\psi_0 e^{-\bar{\psi}_0 \psi_0} \sum_n \langle \zeta \psi_0 | e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle \langle n | \psi_0 \rangle \\ &= \int d\bar{\psi}_0 d\psi_0 e^{-\bar{\psi}_0 \psi_0} \left\langle \zeta \psi_0 \left| e^{-\beta(\hat{H} - \mu \hat{N})} \sum_n |n\rangle \langle n| \right| \psi_0 \right\rangle \\ &= \int d\bar{\psi}_0 d\psi_0 e^{-\bar{\psi}_0 \psi_0} \langle \zeta \psi_0 | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi_0 \rangle , \end{aligned} \quad (13)$$

where in the second step we commute $\langle n | \psi_0 \rangle$ through $\langle \psi_0 | e^{-\beta(\hat{H} - \mu \hat{N})} | n \rangle$ which in the case of Grassmann numbers results in a minus sign. Notice that the index 0 does not correspond to i , the spatial index. It represents the fact that this is the zeroth time we use the resolution

¹Notice 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., at state $ketn$ after a time $t = i\hbar\beta$, which, as you know, can be written as a Feynman path integral

of the identity (as we will use it M more times soon).

The second step is to evaluate the matrix element of the imaginary-time evolution operator: $\langle \zeta \psi_0 | e^{-\beta(\hat{H}-\mu\hat{N})} | \psi_0 \rangle$. To do so we divide the imaginary-time evolution operator into M small steps of imaginary-time δ :

$$e^{-\beta(\hat{H}-\mu\hat{N})} = \left[e^{-\delta(\hat{H}-\mu\hat{N})} \right]^M = \underbrace{\left[e^{-\delta(\hat{H}-\mu\hat{N})} \right] \left[e^{-\delta(\hat{H}-\mu\hat{N})} \right] \dots \left[e^{-\delta(\hat{H}-\mu\hat{N})} \right]}_{M \text{ times}} \quad (14)$$

where $\delta = \beta/M$. We then insert $M - 1$ resolutions of identity, one between each two exponent, inside the imaginary-time evolution operator matrix element, like so:

$$\begin{aligned} \langle \zeta \psi_0 | e^{-\beta(\hat{H}-\mu\hat{N})} | \psi_0 \rangle &= \int \prod_{m=1}^{M-1} d\bar{\psi}_m d\psi_m e^{-\sum_m \bar{\psi}_m \psi_m} \times \\ &\times \langle \zeta \psi_0 \equiv \psi_M | e^{-\delta(\hat{H}-\mu\hat{N})} | \psi_{M-1} \rangle \langle \psi_{M-1} | e^{-\delta(\hat{H}-\mu\hat{N})} | \psi_{M-2} \rangle \dots \langle \psi_1 | e^{-\delta(\hat{H}-\mu\hat{N})} | \psi_0 \rangle, \end{aligned} \quad (15)$$

where for convenience we have given $\zeta \psi_0$ another name, ψ_M . Since δ is small we can expand the exponents to first order in δ to write the matrix elements as:

$$\begin{aligned} \langle \psi_{m+1} | e^{-\delta(\hat{H}-\mu\hat{N})} | \psi_m \rangle &\approx \langle \psi_{m+1} | 1 - \delta (\hat{H} - \mu\hat{N}) | \psi_m \rangle \\ &= \langle \psi_{m+1} | \psi_m \rangle [1 - \delta (H[\bar{\psi}_{m+1}, \psi_m] - \mu N[\bar{\psi}_{m+1}, \psi_m])] \\ &\approx e^{\bar{\psi}_{m+1} \psi_m - \delta (H[\bar{\psi}_{m+1}, \psi_m] - \mu N[\bar{\psi}_{m+1}, \psi_m])} \end{aligned} \quad (16)$$

where we have defined $H[\bar{\psi}_{m+1}, \psi_m] \equiv \frac{\langle \psi_{m+1} | \hat{H} | \psi_m \rangle}{\langle \psi_{m+1} | \psi_m \rangle}$ and $N[\bar{\psi}_{m+1}, \psi_m] \equiv \frac{\langle \psi_{m+1} | \hat{N} | \psi_m \rangle}{\langle \psi_{m+1} | \psi_m \rangle}$. Plugging these into all matrix elements in Eq.(15) and then the result into Eq.(13) we get:

$$\mathcal{Z} = \int \prod_{m=0}^{M-1} d\bar{\psi}_m d\psi_m e^{-\delta \sum_{m=0}^{M-1} \left\{ \left(\frac{\bar{\psi}_m - \bar{\psi}_{m+1}}{\delta} \right) \psi_m + H[\bar{\psi}_{m+1}, \psi_m] - \mu N[\bar{\psi}_{m+1}, \psi_m] \right\}}, \quad (17)$$

and we emphasize again that ψ_M is just another name for $\zeta \psi_0$.

The final step is to take the $M \rightarrow \infty$ ($\delta \rightarrow 0$) limit and obtain

$$\mathcal{Z} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-\int_0^\beta d\tau (\bar{\psi} \partial_\tau \psi + H[\bar{\psi}, \psi] - \mu N[\bar{\psi}, \psi])} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-\mathcal{S}[\bar{\psi}, \psi]}, \quad (18)$$

where the measure is defined as

$$\mathcal{D}[\bar{\psi}, \psi] \equiv \lim_{M \rightarrow \infty} \prod_{m=0}^M d\bar{\psi}_m d\psi_m = \lim_{M \rightarrow \infty} \prod_{m=0}^M \prod_i \frac{d\bar{\psi}_{i,m} d\psi_{i,m}}{\pi^{\frac{\zeta+1}{2}}}, \quad (19)$$

and the integration is to be carried over fields $\psi(\tau)$ satisfying the boundary condition $\psi(\beta) = \zeta\psi(0)$ (and corresponding condition on $\bar{\psi}$). It is very important to note that by neglecting the time derivative term we reduce 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 interacting theories with the actions of the following form:

$$\mathcal{S} = \int_0^\beta d\tau \left[\sum_{i,j} \bar{\psi}_i [(\partial_\tau - \mu) \delta_{i,j} + h_{i,j}] \psi_j + \sum_{i,j,k,l} V_{i,j,k,l} \bar{\psi}_i(\tau) \bar{\psi}_j(\tau) \psi_k(\tau) \psi_l(\tau) \right]. \quad (20)$$

To make progress on computing things with the path integral we usually transform to the Fourier basis where the derivative operators are diagonal. This procedure applies also for the imaginary time derivative, where one transforms

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{n=-\infty}^{\infty} \psi_n e^{-i\omega_n \tau}, \quad (21)$$

where in order to obey the boundary conditions $\psi(0) = \zeta\psi(\beta)$ we choose the following frequencies:

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} & \text{Bosons} \\ \frac{(2n+1)\pi}{\beta} & \text{Fermion} \end{cases}. \quad (22)$$

These imaginary-time frequencies are known as *Matsubara frequencies*. Plugging the transformation into the action, and using $\int_0^\beta d\tau e^{-i(\omega_n - \omega_m)\tau} = \delta_{n,m}$, we indeed diagonalize the imaginary-time derivative to get

$$\mathcal{S} = \sum_{n,i,j} \bar{\psi}_{i,n} [(-i\omega_n - \mu) \delta_{i,j} + h_{i,j}] \psi_{j,n}$$

$$+ \frac{1}{\beta} \sum_{i,j,k,l,n_i} V_{i,j,k,l} \bar{\psi}_{i,n_1} \bar{\psi}_{j,n_2} \psi_{k,n_3} \psi_{l,n_4} \delta_{n_1+n_2,n_3+n_4}. \quad (23)$$

However, summing over Matsubara frequencies is a whole story by itself. You will see an example in the exercise. I want to note that in the limit of zero temperature ($\beta \rightarrow \infty$) the sum becomes a simple integral $\frac{1}{\beta} \sum_n \rightarrow \int \frac{d\omega}{2\pi}$.

3 The Hubbard-Stratonovich transformation

In this section we will learn a general method to relate a Ginzburg-Landau (phenomenological) theory to the underlying microscopic theory. For example we consider the GL theory of a ferromagnet, which is described by the magnetization vector \vec{m} . The GL free energy in this example is given by:

$$F_{GL} = \int d^3x \left[\alpha \vec{m}^2 + \beta \vec{m}^4 - a \vec{m} \nabla^2 \vec{m} \right], \quad (24)$$

where, as you know, α is a function of the temperature and when $\alpha < 0$ the magnetization \vec{m} obtains an expectation value (spontaneous symmetry breaking) and the system becomes ferromagnetically ordered.

To see how to relate this theory to an underlying microscopic theory let us consider the action of fermions (electrons) with point contact density-density interaction:

$$\mathcal{Z} = \mathcal{D} [\bar{\psi}, \psi] e^{-\mathcal{S}}, \quad (25a)$$

$$\mathcal{S} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s + g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right]. \quad (25b)$$

The interaction term may be reorganized in the following manner: $\bar{\psi}_\uparrow(x) \bar{\psi}_\downarrow(x) \psi_\downarrow(x) \psi_\uparrow(x) = -\vec{s}(x) \cdot \vec{s}(x)$, where $\vec{s}(x) = \frac{1}{2} \bar{\psi}_s \sigma_{ss'} \psi_{s'}$, and thus the action is equivalently given by:

$$\mathcal{S} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s - g \vec{s} \cdot \vec{s} \right]. \quad (26)$$

We are now ready to perform the Hubbard-Stratonovich transformation which relies on the

following central identity:

$$1 = \int \mathcal{D}[\vec{m}] \exp \left[-g \int_0^\beta d\tau d^3x (\vec{m} - \vec{s})^2 \right] , \quad (27)$$

which is possible since we can shift \vec{s} away from the “action” and choose the measure in a way that takes care of all constants and parameters. The transformation is done by multiplying the partition function \mathcal{Z} by 1 which is then expressed in this way. We find a new, equivalent, formulation of the theory. Namely,

$$\mathcal{Z} = \int \mathcal{D}[\bar{\psi}, \psi, \vec{m}] e^{-\mathcal{S}_{\text{HS}}} , \quad (28a)$$

$$\mathcal{S}_{\text{HS}} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s - 2g\vec{m} \cdot \vec{s} + g\vec{m}^2 \right] . \quad (28b)$$

Notice that the HS action above resembles a mean-field decoupling of the interaction term. To see this substitute $\vec{s} = \vec{M} + \delta\vec{s}$ in the interaction term, where \vec{M} is the mean-field value and $\delta\vec{s}$ are small fluctuations, neglect terms of order $O(\delta\vec{s}^2)$, and re-express with \vec{M} and \vec{s} like so:

$$-g\vec{s} \cdot \vec{s} = -g(\vec{M} + \delta\vec{s})(\vec{M} + \delta\vec{s}) \approx -g\vec{M}^2 - 2g\vec{M} \cdot \delta\vec{s} = -2g\vec{M} \cdot \vec{s} + g\vec{M}^2 \quad (29)$$

However, there is a crucial difference in that \vec{M} is a mean-field with a single value whereas the field \vec{m} fluctuates and we integrate over all its possible configurations. Actually, equation (28a) is exact, as we made no approximations in deriving it. As you will see in the exercise the saddle point approximation of the HS theory gives the self-consistent mean-field approximation obtained from a variational method. This observation suggests that the field \vec{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 (28a) to obtain an effective theory for the magnetization field \vec{m} . The standard way is to “integrate out” the Fermions. Since the action for the fermions is quadratic this is easy to do, and because the \vec{m} field couples

to them doing so will generate new terms for it. First let us rewrite the theory as

$$\mathcal{S}_{\text{HS}} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\underbrace{\left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right)}_{G^{-1}} \delta_{ss'} - \underbrace{g\vec{m} \cdot \sigma_{ss'}}_X \right) \psi_{s'} + g\vec{m}^2 \right]. \quad (30)$$

Remember that we know how to perform Gaussian fermionic (Grassman) integrals, so, denoting $A = G^{-1} - X[\vec{m}]$, we get

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}[\vec{m}] \det(A) e^{-g \int_0^\beta d\tau d^3x \vec{m}^2} \\ &= \int \mathcal{D}[\vec{m}] e^{-g \int_0^\beta d\tau d^3x \vec{m}^2 + \log[\det(A)]} \\ &= \int \mathcal{D}[\vec{m}] e^{-g \int_0^\beta d\tau d^3x \vec{m}^2 + \text{Tr}[\log(A)]}. \end{aligned} \quad (31)$$

The trace of the logarithm can be expanded perturbatively in small $X[\vec{m}]$ in the following manner:

$$\begin{aligned} \text{Tr}[\log(A)] &= \text{Tr}[\log(G^{-1} - X[\vec{m}])] = \text{Tr}[\log(G^{-1})] + \text{Tr}[\log(1 - GX[\vec{m}])] \\ &= \text{Tr}[\log(G^{-1})] + \text{Tr}\left(-GX[\vec{m}] + \frac{1}{2}GX[\vec{m}]GX[\vec{m}] + \dots\right). \end{aligned} \quad (32)$$

Since $X[\vec{m}]$ is linear in \vec{m} each order in X gives the corresponding order in the Ginzburg-Landau theory. The first order term vanishes, as it must due to symmetry. The second order term, if expanded in momentum basis, gives the following quadratic term:

$$\begin{aligned} \frac{1}{2} \text{Tr}(GX[\vec{m}]GX[\vec{m}]) &= \frac{1}{2} \sum_{\vec{q}, n, s} \langle \vec{q}, n, s | GX[\vec{m}]GX[\vec{m}] | \vec{q}, n, s \rangle \\ &= -g^2 \sum_{\vec{q}, n} \Pi(\vec{q}, \omega_n) |\vec{m}(\vec{q}, \omega_n)|^2, \end{aligned} \quad (33)$$

where

$$\Pi(\vec{q}, \omega_n) = \frac{1}{\beta V} \sum_{\vec{k}, m} \left[\frac{1}{-i\omega_m + \frac{\vec{k}^2}{2m} - \mu} \right] \left[\frac{1}{-i(\omega_m + \omega_n) + \frac{(\vec{k} + \vec{q})^2}{2m} - \mu} \right], \quad (34)$$

and we have used the facts that G is diagonal in spin space and the Pauli matrices are

traceless. We can expand this in small \vec{q} and get the parameters of the Ginzburg-Landau theory:

$$\alpha = g - g^2 \Pi(0, 0) \ , \quad (35)$$

which indeed depends on temperature (through Π) as expected, and

$$a = \frac{g^2}{2} \left(\frac{\partial^2 \Pi(\vec{q}, 0)}{\partial \vec{q}^2} \right) \Big|_{\vec{q}=0} . \quad (36)$$

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