Tutorials for "Concepts of condensed matter physics"

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Chapter 1

Tutorial #1 - many-body path-integral formalism and the Hubbard-Stratonovich transformation

1.1 References for this tutorial

Altland & Simons Chapter 4 & 6.
Mahan

1.2 Introduction

In this tutorial we have two objectives: (i) *Imaginary time coherent state path integral formalism* - to prove the identity (1.9). The motivation will be to show that quantum averages of many-body systems in thermal equilibrium can be computed using Feynman's path integral formalism. (ii) *The Hubbard-Stratonovich transformation* - To provide a rigors formalism in which the phenomenological Ginzburg-Landau (GL) theory can be related to it's underlying microscopic theory theory. Here the motivation is obvious.

1.3 (i) Coherent-state path-integral in imaginary time

Before getting to the path integral itself let us quickly go over a few basic properties of coherent states. A coherent state is an eigenstate of an annihilation operator a

$$|\psi\rangle \equiv e^{\zeta\psi a^\dagger}|0\rangle \tag{1.1}$$

where $\zeta = 1$ ($\zeta = -1$) for Bosons (Fermions).

1.3.1 c-numbers

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

$$\langle\psi_1|\psi_2\rangle = e^{\bar{\psi}_1\psi_2} \tag{1.2}$$

The second is the resolution of identity which follows directly from (1.2)

$$\mathbb{1} = \int d\bar{\psi}d\psi\, e^{-\bar{\psi}\psi}\,|\psi\rangle\langle\psi| \tag{1.3}$$

Generally ψ is a vector with a discrete set of components ψ_i corresponding to the underlying Fock space. Thus it's continuum limit will be a field, for example $\psi(x)$. Additionally, $\bar{\psi}\psi \equiv \sum_i \bar{\psi}_i\psi_i$ 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 $\bar{\psi}$

$$\int d\bar{\psi}d\psi\, e^{-\bar{\psi}A\psi} = \frac{1}{|A|} \tag{1.4}$$

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

1.3.2 Grassmann numbers

If the operator a describes a fermionic excitation things become a bit more complected. This is because the eigen value ψ can not be taken to be an ordinary complex number (it is easy to show that if the a_i's anti-commute amongst themselves and ψ_i are c-numbers then $\langle\psi|a_i a_j|\psi\rangle = 0$ directly follows). To make sense we need special numbers that anti-commute, these are known as Grassmann numbers:

$$\psi_i\psi_j = -\psi_j\psi_i \tag{1.5}$$

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

$$\int d\psi = 0 \;\; ; \;\; \int d\psi\,\psi = 1 \tag{1.6}$$

and

$$\partial_\psi \psi = 1 \tag{1.7}$$

The overlap between two coherent states and the resolution of identity remain in the form of (1.2) and (1.3). The Gaussian integral on the other hand is significantly different

$$\int d\bar{\psi} d\psi \, e^{-\bar{\psi} A \psi} = |A| \tag{1.8}$$

where A can be any matrix. Exercise: use (1.5) and (1.6) to prove (1.8).

1.4 Imaginary-time many-body path-integrals

In what follows we will prove the following identity

$$\mathcal{Z} = \mathrm{Tr} e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} = \int \mathcal{D}[\psi,\bar{\psi}] e^{-\int_0^\beta d\tau\left(\bar{\psi}\partial_\tau\psi+\mathcal{H}[\bar{\psi},\psi]-\mu N[\bar{\psi},\psi]\right)} \tag{1.9}$$

where $\mathcal{H}$ and N are the Hamiltonian and particle number respectively and $\psi, \bar{\psi}$ are c-numbers (Grassmann variables) in the case that the particles have Bosonic (Fermionic) mutual statistics. 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

$$\langle \hat{A} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi,\bar{\psi}] A[\psi,\bar{\psi}] e^{-\int_0^\beta d\tau\left(\bar{\psi}\partial_\tau\psi+\mathcal{H}[\bar{\psi},\psi]-\mu N[\bar{\psi},\psi]\right)} \tag{1.10}$$

Question: why did we choose a coherent state path integral? and not say a real space or momentum path integral.

Let start with the definition of the trace

$$\mathcal{Z} = \mathrm{Tr} e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} = \sum_n \langle n| e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} |n\rangle \tag{1.11}$$

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 casted to 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 (1.3) into equation (1.11)

$$\mathcal{Z} = \int d\bar{\psi} d\psi \, e^{-\bar{\psi}\psi} \sum_n \langle n|\psi\rangle \langle\psi| e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} |n\rangle \tag{1.12}$$

We can sum over n using the resolution of identity $\mathbb{1} = \sum_n |n\rangle\langle n|$ but we first need to commute $\langle n|\psi\rangle$ with another. In the case of bosonic particles this is just a number and it commutes with anything. In the case of fermions it is a Grassmann number and therefore collects a minus sign which can be absorbed into the coherent state

$$\mathcal{Z} = \frac{1}{\pi}\int d\bar{\psi}d\psi\, e^{-\bar{\psi}\psi}\,\langle\zeta\psi|e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}|\psi\rangle \tag{1.13}$$

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

$$e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} = \left[e^{-\delta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}\right]^M \tag{1.14}$$

where $\delta = \beta/M$. In the third step we insert M resolutions of identity in the expectation value in equation (1.13)

$$\langle\zeta\psi|[e^{-\delta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}]^M|\psi\rangle = \int\prod_{m=1}^{M} d\bar{\psi}^m d\psi^m e^{-\sum_m\bar{\psi}^m\psi^m}\times \tag{1.15}$$

$$\langle\zeta\psi|\psi^1\rangle\langle\psi^1|e^{-\delta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}|\psi^2\rangle\langle\psi^2|e^{-\delta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}|\psi^3\rangle\langle\psi^3|...|\psi^M\rangle\langle\psi^M|e^{-\delta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}|\psi\rangle$$

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

where we have denoted $\psi^0 = \zeta\psi^{M+1} = \psi$. Now if we insert this expression in (1.13) we get

$$\mathcal{Z} = \int_{\psi^0=\zeta\psi^M;\bar{\psi}^0=\zeta\bar{\psi}^M}\prod_{m=0}^{M} d\bar{\psi}^m d\psi^m e^{-\delta\sum_{m=0}^{M}\left[\left(\frac{\bar{\psi}^m-\bar{\psi}^{m+1}}{\delta}\right)\psi^m+\mathcal{H}[\bar{\psi}^m,\psi^{m+1}]-\mu N[\bar{\psi}^m,\psi^{m+1}]\right]} \tag{1.16}$$

Finally, the fourth step, we take $M\to\infty$ and obtain (1.9),

$$\mathcal{Z} = \int\mathcal{D}[\psi,\bar{\psi}]e^{-\int_0^\beta d\tau\left(\bar{\psi}\partial_\tau\psi+\mathcal{H}[\bar{\psi},\psi]-\mu N[\bar{\psi},\psi]\right)} \tag{1.17}$$

where

$$\mathcal{D}[\bar{\psi},\psi] \equiv \lim_{M\to\infty}\prod_{m=0}^{M} d\bar{\psi}^m\psi^m \tag{1.18}$$

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 casted to fields ψ_i and $\bar{\psi}_i$ which always have trivial (anti-)commutation relations.

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

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_\nu \psi(\nu) e^{-i\nu\tau} \tag{1.19}$$

in which case the action takes the form

$$\mathcal{S} = \frac{1}{\beta} \sum_n \left(-i\nu\bar{\psi}\psi + \mathcal{H}[\bar{\psi}, \psi] - \mu N[\bar{\psi}, \psi] \right) \tag{1.20}$$

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

$$\nu_n = \begin{cases} \frac{2n\pi}{\beta} & \text{Bosons} \\ \frac{(2n+1)\pi}{\beta} & \text{Fermions} \end{cases} \tag{1.21}$$

These imaginary-time frequencies are known as *Matsubara frequencies*. Summing over them is a whole story to itself which will not be discussed in this course. I will only state the identity

$$\frac{\zeta}{\beta} \sum_n \frac{1}{-i\nu_n + x} = \begin{cases} n_B(x) & \text{Bosons} \\ n_F(x) & \text{Fermions} \end{cases} \tag{1.22}$$

where $n_B(x)$ ($n_F(x)$) is the Bose (Fermi) distribution function at temperature β^{-1}. I will also note that in the limit of zero temperature ($\beta \to \infty$) the sum becomes a simple integral $\frac{1}{\beta}\sum_{\nu_n} \to \int_{-\infty}^{\infty} \frac{d\nu}{2\pi}$. Students that wish to understand how to perform these sums should refer to Altland & Simons pages 169-172 or the book by Mahan.

1.5 The Hubbard-Stratonovich transformation

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

$$\mathcal{F}_{GL} = \int d^3x \left[-\alpha \boldsymbol{m} \nabla^2 \boldsymbol{m} + am^2 + \beta m^4 \right] \tag{1.23}$$

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

$$\mathcal{Z} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-\mathcal{S}} \tag{1.24}$$

$$\mathcal{S} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s + g\, \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right] \quad = \tag{1.25}$$

Notice that the local interaction may reorganized in the following manner

$$\bar{\psi}_\uparrow(x) \bar{\psi}_\downarrow(x) \psi_\downarrow(x) \psi_\uparrow(x) = -\boldsymbol{s}(x) \cdot \boldsymbol{s}(x) \tag{1.26}$$

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

$$\mathcal{S} = \int_0^\beta d\tau d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s - g s^2 \right] \quad = \tag{1.27}$$

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

$$\begin{aligned} &\int \mathcal{D}[\boldsymbol{m}] \exp\left[-\int_0^\beta d\tau \int d^3x \left(m^2 - 2\boldsymbol{m} \cdot \boldsymbol{s} \right) \right] \\ &= \underbrace{\int \mathcal{D}[\boldsymbol{m}] \exp\left[-\int_0^\beta d\tau \int d^3x |\boldsymbol{m} - \boldsymbol{s}|^2 \right]}_{N} \exp\left[\int_0^\beta d\tau \int d^3x\, s^2 \right] \\ &= N \exp\left[\int_0^\beta d\tau \int d^3x\, s^2 \right] \end{aligned} \tag{1.28}$$

Thus, equation (1.24) may be equivalently written as follows

$$\mathcal{Z} = \frac{1}{N} \int \mathcal{D}[\bar{\psi}, \psi, \boldsymbol{m}] e^{-\mathcal{S}_{HS}} \tag{1.29}$$

where

$$\mathcal{S}_{HS} = \int_0^\beta d\tau \int d^3x \left[\sum_{s=\uparrow\downarrow} \bar{\psi}_s \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_s - 2g\boldsymbol{m} \cdot \boldsymbol{s} + g m^2 \right] \tag{1.30}$$

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

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

However, there is a crucial difference: $\boldsymbol{M}$ is a mean-field with a single value whereas the field $\boldsymbol{m}$ fluctuates and we integrate over all possible paths of this field. Actually, equation (1.29) 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.

Finally, let us discuss how we can use the HS theory (1.29) to obtain an effective theory for the "magnetization" field $\boldsymbol{m}$. The standard way is to integrate over the Fermions. First let us rewrite the theory as follows

$$\mathcal{S}_{HS} = \int_0^\beta d\tau \int d^3x \left[\sum_{ss'} \bar{\psi}_s \left[\underbrace{\left(\partial_\tau - \frac{\nabla^2}{2m} - \mu\right)\delta_{ss'}}_{\mathcal{G}^{-1}} - \underbrace{g\boldsymbol{m}\cdot\boldsymbol{\sigma}_{ss'}}_{X} \right] \psi'_s + gm^2 \right] \tag{1.31}$$

Therefore formally the fermionic part of the path integral has the form

$$\int d\bar{\psi} d\psi \, e^{-\bar{\psi}A\psi} \tag{1.32}$$

where $A = \mathcal{G}^{-1} - X[\boldsymbol{m}]$. Thus using (1.8) we can perform the integral over the fermions which gives

$$\mathcal{Z} = \frac{1}{N}\int \mathcal{D}[\boldsymbol{m}]|A|\, e^{-gm^2} = \frac{1}{N}\int \mathcal{D}[\boldsymbol{m}]\, e^{-gm^2+\log|A|} = \frac{1}{N}\int \mathcal{D}[\boldsymbol{m}]\, e^{-gm^2+\mathrm{Tr}\,\log A} \tag{1.33}$$

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

$$\begin{aligned} \mathrm{Tr}\,\log A &= \mathrm{Tr}\,\log(\mathcal{G}^{-1} - X) = \mathrm{Tr}\log\mathcal{G}^{-1} + \mathrm{Tr}\,\log(1-\mathcal{G}X) \\ &= \mathrm{Tr}\log\mathcal{G}^{-1} + \mathrm{Tr}\left[-\mathcal{G}X + \frac{1}{2}\mathcal{G}X\mathcal{G}X + \ldots\right] \end{aligned}$$

Now since X is linear in $\boldsymbol{m}$ each order gives the corresponding order in the Ginzburg-Landau theory. For example the second order term gives the quadratic term (at zero temperature)

$$\frac{1}{2}\mathrm{Tr}[\mathcal{G}X\mathcal{G}X] = \frac{g^2}{\beta\Omega}\sum_{\boldsymbol{q}\omega} \Pi(\boldsymbol{q},\omega)\boldsymbol{m}_{\boldsymbol{q}}(\omega)\boldsymbol{m}_{-\boldsymbol{q}}(-\omega) \tag{1.34}$$

where

$$\Pi(\omega, \boldsymbol{q}) = \frac{1}{\beta\Omega} \sum_{\boldsymbol{k}\nu} \frac{1}{-i\nu + \frac{k^2}{2m} - \mu} \frac{1}{-i(\nu+\omega) + \frac{(\boldsymbol{k}+\boldsymbol{q})^2}{2m} - \mu} \tag{1.35}$$

and we have used the fact that $\mathcal{G}$ is diagonal in spin space and that the Pauli matrices are traceless. The parameters of (1.23) are then given by

$$a = \Pi(0,0) \tag{1.36}$$

and

$$\alpha = \frac{1}{2} \left(\frac{\partial^2 \Pi(q,0)}{\partial q} \right)_{q=0} \tag{1.37}$$

Of course β will derive from the higher order term with four powers of X.