7. FUNCTIONAL INTEGRALS

In first quantization, the Feynmann path integral is an integral over all coordinates. The coordinates are operators in the Hamiltonian formalism. In the path integral case, the argument of the exponential is the action in units of \( \hbar \). By analogy, in second quantization, we want a path integral where the argument of the exponential is the action and the integrals are over fields. For bosons, it suffices to work in the coherent state basis. Coherent states for bosons are the analogs of classical fields. What are coherent states for fermions? This is what we set to do first. Then the functional integral follows naturally.

7.1 Grassmann variables for fermions

7.1.1 Fermion coherent states

We wish to compute the partition function for time-ordered products with imaginary-time dependent Hamiltonians. This occurs when one does perturbation theory, or with source fields. To rewrite the partition function, or expectation values, it is convenient to use a basis where the partition function is expressed as a functional integral. In the case of bosons, one uses coherent states. In the case of fermions, by analogy, one can define fermion coherent states. For simplicity, we work with spinless fermions.

Let \( c \) be a fermion destruction operator, then \( c |0\rangle = 0 \) while for the fermion coherent state \( \eta \), we have

\[
    c |\eta\rangle = \eta |\eta\rangle .
\]  

(7.1)

Since \( c_1 c_2 |\eta_1, \eta_2\rangle = -c_2 c_1 |\eta_1, \eta_2\rangle \) the eigenvalues \( \eta \) must be numbers that anticommute. Namely,

\[
    \{\eta_1, \eta_2\} = 0 .
\]  

(7.2)

Since Grassmann numbers occur only inside time-ordered products, it turns out that it suffices to define the adjoint in such a way that it also anticommutes, there is no delta function:

\[
    \{\eta, \eta^\dagger\} = 0 .
\]  

(7.3)

Given the definition of Grassmann numbers, one can write an explicit definition of fermion coherent states in the Fock basis is we add the definition that Grassmann numbers and fermion operators also anticommute:

\[
    |\eta\rangle = (1 - \eta c^\dagger) |0\rangle.
\]  

(7.4)

Given that \( \eta^2 = 0 \), one can verify the defining property \( c |\eta\rangle = \eta |\eta\rangle \) Eq.(7.1):

\[
    c |\eta\rangle = c |0\rangle + \eta c c^\dagger |0\rangle = \eta |0\rangle = \eta (1 - \eta c^\dagger) |0\rangle = \eta |\eta\rangle .
\]  

(7.5)
7.1.2 Grassmann integrals

In the case of bosons, the amplitude of a coherent state is arbitrary. For fermions, we imagine something analog. We must define then Grassmann integrals. To have meaning as integrals, these must satisfy properties such as

\[ \int d\eta f (\eta + \xi) = \int d\eta f (\eta) \]  
(7.6)

where \( \xi \) is another Grassmann number. The most general function of a Grassmann variable is \( f (\eta) = a + b\eta \) since \( \eta^2 = 0 \). Hence, the above property is satisfied if \( \int dq b\xi = 0 \), which implies

\[ \int d\eta = 0. \]  
(7.7)

For derivatives and integrals to be coherent, the formula for integration by parts is also satisfied with the above definition (as if \( f \) vanished at infinity)

\[ \int d\eta \frac{df}{d\eta} = 0. \]  
(7.8)

Linearity

\[ \int d\eta (af (\eta) + bg (\eta)) = \int d\eta af (\eta) + \int d\eta bg (\eta) \]

will be satisfied as long as \( \int d\eta \eta \) is a number. The choice

\[ \int d\eta \eta = 1 \]  
(7.10)

is convenient. The last property is consistent with the fact that the product of two Grassmann numbers is an ordinary number. In the end, note that the formula for integration looks the same as the formula for differentiation. The two rules Eqs.7.7 and 7.10 are all we need to remember.

7.1.3 Grassmann Gaussian integrals

Let us practice with the integral we will meet all the time, the analog of the Gaussian integral. With the above rules for integration, and \( e^{-\eta^\dagger \eta} = 1 - \eta^\dagger \eta \) that follows from \( \eta^2 = 0 \), we find

\[ \int d\eta^\dagger \int d\eta e^{-\eta^\dagger a\eta} = \int d\eta^\dagger \int d\eta (1 - \eta^\dagger a\eta) = a = \exp (\log (a)) \]  
(7.11)

where \( a \) is an ordinary number. If we have two Grassman variables,

\[ \int d\eta_1 \int d\eta_2^\dagger e^{-\eta_1^\dagger a_1 \eta_1} \int d\eta_2 \int d\eta_2^\dagger e^{-\eta_2^\dagger a_2 \eta_2} = \]

\[ \int d\eta_1 \int d\eta_1^\dagger \int d\eta_2 \int d\eta_2^\dagger e^{-\eta_1^\dagger a_1 \eta_1} e^{-\eta_2^\dagger a_2 \eta_2} = a_1 a_2 \]  
(7.12)

\[ = \exp \left( \log a_1 + \log a_2 \right) \]

(7.13)

The quantity \( a_1 a_2 \) is the determinant of the diagonal matrix with \( a_1 \) and \( a_2 \) on the diagonal. In a general basis then we write in matrix notation

\[ \prod_i \int d\eta_i \int d\eta_i^\dagger e^{-\eta_i^\dagger A \eta} = \det (A) = \exp \left( \text{Tr} \log (A) \right) \]  
(7.14)

FUNCTIONAL INTEGRALS
The last equalities follow by using the fact that the determinant and the trace are both basis independent. We abbreviate further the notation with the definition of the integration measure

\[ \int D\eta^\dagger \int D\eta e^{-\eta^\dagger A \eta} \equiv \prod_i \int d\eta_i \int d\eta_i^\dagger e^{-\eta_i^\dagger A \eta_i}. \] (7.15)

There is another gaussian integral to do that is simple and that will allow us to use source fields to our benefit. Defining the Grassman source fields \( J \) and \( J^\dagger \), we can use what we know about shifting the origin of integration, Eq. (7.6), and obtain

\[ \int d\eta^\dagger \int d\eta e^{-\eta^\dagger a \eta - \eta^\dagger J - J^\dagger \eta} = \int d\eta^\dagger \int d\eta e^{-(\eta^\dagger + J^\dagger a^{-1})a(\eta + a^{-1} J) + J^\dagger a^{-1} J}. \] (7.16)

The generalization to integrals over many Grassmann variables gives

\[ \int D\eta^\dagger \int D\eta e^{-\eta^\dagger A \eta - \eta^\dagger J - J^\dagger \eta} = \int D\eta^\dagger \int D\eta e^{-(\eta^\dagger + J^\dagger A^{-1})\eta (\eta + A^{-1} J) + (J^\dagger A^{-1} J)} = \det(A) \exp(J^\dagger A^{-1} J). \] (7.18)

We will be able to use this result to obtain Green’s functions or multipoint functions from functional derivatives with respect to \( J \).

### 7.1.4 Completeness relation and trace formula

To find the expression for the partition function, we will need the completeness relation. From the last result of the previous section, one can verify the following closure formula by applying it successively on \( |\eta\rangle \) and on \( c^\dagger \langle 0| \) :

\[ \int d\eta^\dagger \int d\eta e^{-\eta^\dagger \eta} |\eta\rangle \langle \eta| = \int d\eta^\dagger \int d\eta (1 - \eta^\dagger \eta) |\eta\rangle \langle \eta| = I. \] (7.19)

Take a single state that can be empty or occupied. The trace of an operator \( O \) can be written as follows,

\[ \text{Tr}[O] = \int d\eta^\dagger \int d\eta e^{-\eta^\dagger \eta} (-\eta|O|\eta). \] (7.20)

The minus sign reflects the antiperiodicity that we encounter with fermions. To prove the above formula, it suffices to use the definition of the fermionic coherent state Eq. (7.4). Indeed,

\[ \int d\eta^\dagger \int d\eta e^{-\eta^\dagger \eta} (-\eta|O|\eta) = \int d\eta^\dagger \int d\eta e^{-\eta^\dagger \eta} (0| (1 + c\eta^\dagger) O (1 - \eta c^\dagger) |0) \]
\[ = \int d\eta^\dagger \int d\eta (1 - \eta^\dagger \eta) (0| (1 + c\eta^\dagger) O (1 - \eta c^\dagger) |0) \]
\[ = \int d\eta^\dagger \int d\eta (1 - \eta^\dagger \eta) \left( \langle 0| O |0\rangle - \langle 0| c\eta^\dagger O \eta c^\dagger |0\rangle \right) \]
\[ = \int d\eta^\dagger \int d\eta (1 - \eta^\dagger \eta) \left( \langle 0| O |0\rangle + \eta^\dagger \eta \langle 0| cOc^\dagger |0\rangle \right) \]
\[ = \langle 0| O |0\rangle + \langle 1| O |1\rangle \] (7.21)
In the next to last equation, we assumed that $O$ contains an even number of fermion operators so that
\[ \eta O = -O \eta. \]  
(7.22)

The set is overcomplete since using the definition in terms of Fock states Eq. (7.4), one finds
\[ \langle \eta_1 | \eta_2 \rangle = \langle \eta | (1 - \eta_1^\dagger \eta_1) (1 - \eta_2 \eta_2^\dagger) | 0 \rangle = 1 + \eta_1^\dagger \eta_2 = e^{\eta_1^\dagger \eta_2}. \]  
(7.23)

7.1.5 The functional integral for a single fermion

For spinless fermions whose Hamiltonian is given by $H = \sum_i \varepsilon_i c_i^\dagger c_i$, the partition function is
\[ Z = \text{Tr} (\exp (-\beta H)) = \prod_i (1 + e^{-\beta \varepsilon_i}) = \det (1 + e^{-\beta \varepsilon}) \]  
(7.24)

where $\varepsilon$ is the diagonal matrix. The expression remains valid in an arbitrary basis. What is the generalization of this result when $H$ depends on $\tau$ and we want a time-ordered product
\[ Z = \text{Tr} \left( T_{\tau} \exp \left( -\beta \int_0^\beta d\tau H(\tau) \right) \right). \]  
(7.25)

We can work this out in the usual operator formalism. With Grassmann variables, we need to suffer first, but then the calculations are easy and formally very close to those for bosons.

Let us start with a single fermion state, so that $H = \varepsilon c^\dagger c$.

Then, we express the trace in the coherent fermion basis. In that basis, we do not know how to compute $e^{-\beta H} | \eta \rangle$ since the expansion of the exponential gives an infinite number of terms. We can however use the Trotter decomposition to do a Taylor expansion that will be easy to evaluate in the coherent state basis. The Trotter decomposition is given by
\[ e^{-\beta H} = \lim_{N_\tau \to \infty} \prod_{i=1}^{N_\tau} e^{-\Delta \tau_i H} = \lim_{N_\tau \to \infty} \prod_{i=1}^{N_\tau} (1 - \Delta \tau_i H). \]  
(7.26)

with $\Delta \tau = \beta / N_\tau$. The index $i$ on $\Delta \tau$ is just to allow us to keep track of the different terms. Even if $H$ was time dependent, we could use this approximation in the limit $\Delta \tau \to 0$ because $[\Delta \tau H(\tau_1), \Delta \tau H(\tau_2)] = O(\Delta \tau)^2$ and we will neglect terms of that order. In other words, for $\Delta \tau \to 0$ we can assume that exponentials of sums of operators can be rewritten as a product of exponentials. There is one subtlety. We have many time-slices. Since $N_\tau (\Delta \tau)^2 = \beta \Delta \tau$, it looks as if the error is of order $\Delta \tau$, not $(\Delta \tau)^2$. Fye has shown that the prefactor of $\beta \Delta \tau$ vanishes when one is interested in expectation values of certain kinds of operators. This is basically because the operator in front of $\Delta \tau$ is a commutator and is thus anti-Hermitian. The trace of that anti-hermitian operator vanishes.

Back to our task. Using the trace formula in the coherent state basis Eq.(7.20) and inserting the completeness relation Eq.(7.19) between each term of the product, we can evaluate the exponential in the coherent-state basis. We find, with
the definitions $\eta_\beta = \eta_{N_\tau} = -\eta_0$

\[
Z = \lim_{N_\tau \to \infty} \prod_{i=1}^{N_\tau} \mathcal{D}\eta_i \langle \beta | 1 - \Delta \tau \mathcal{H} c | \eta_{N_\tau-1} \rangle e^{-\eta_{N_\tau-1}^\dagger \eta_{N_\tau-1}^\tau} \langle \eta_{N_\tau-1} | \\
\ldots | \eta_1 \rangle e^{-\eta_1^\dagger \eta_1} \langle \eta_1 | 1 - \Delta \tau_1 c | \eta_0 \rangle
\]

\[
= \lim_{N_\tau \to \infty} \prod_{i=1}^{N_\tau} \mathcal{D}\eta_i \langle \beta | e^{-\eta_N^\dagger \eta_N} \langle \eta_{N_\tau-1} | e^{-\epsilon \eta_{N_\tau-1} \Delta \tau} e^{-\eta_{N_\tau-1}^\dagger \eta_{N_\tau-1}} \langle \eta_{N_\tau-1} | \\
\ldots | \eta_1 \rangle e^{-\eta_1^\dagger \eta_1} \langle \eta_1 | e^{-\epsilon \eta_0} \eta_0 \Delta \tau.
\]

\[
(7.27)
\]

\[
(7.28)
\]

which is a time-ordered product. The overlaps are given by, for example, $e^{-\eta_1^\dagger \eta_1} \langle \eta_1 | \eta_0 \rangle = e^{-\eta_1^\dagger \eta_1 + \eta_1^\dagger \eta_0}$. The above formula is obviously generalizable to a time-dependent Hamiltonian that appears in a time-ordered product. To evaluate this quantity on a computer, we need to first do the integrals over Grassmann variables and express the result in terms of matrices, remembering that the definition of the matrix must be read off the above formula. There is no ambiguity. Recalling that $e^{-\eta_1^\dagger \eta_1} \langle \eta_1 | \eta_0 \rangle = e^{-\eta_1^\dagger \eta_1 + \eta_1^\dagger \eta_0}$, the matrix $A$ that appeared in Eq. (7.14) can be written as

\[
A = \begin{bmatrix}
1 & 0 & 0 & 0 & (1 - \epsilon \Delta \tau) \\
-1 + \epsilon \Delta \tau & 1 & 0 & 0 & 0 \\
0 & -1 + \epsilon \Delta \tau & 1 & \ldots & 0 \\
0 & 0 & \ldots & \ldots & 0 \\
0 & 0 & 0 & -1 + \epsilon \Delta \tau & 1
\end{bmatrix} = -G^{-1}.
\]

\[
(7.29)
\]

In actual computations, it is more accurate to replace $-1 + \epsilon \Delta \tau$ by $-e^{\epsilon \Delta \tau}$. If $\epsilon$ is time dependent, it suffices to replace its value at the appropriate time slice. The above matrix has dimension $N_\tau \times N_\tau$. Labels 0 to $N_\tau - 1$ or 1 to $N_\tau$ can be used. In other words, either time $\tau = 0$ or $\tau = \beta$ can be present as independent labels, but not both. They are related by antiperiodicity.

The continuum limit can also be taken formally. We can combine the exponentials coming from the completeness relation and from the overlap of fermion coherent states as follows

\[
e^{-\eta_1^\dagger \eta_1} \langle \eta_1 | \eta_0 \rangle = e^{-\eta_1^\dagger \eta_1 + \eta_1^\dagger \eta_0} = e^{-\eta_1^\dagger (\eta_1 - \eta_0)} = e^{-\eta_1^\dagger \eta_1^\tau \eta_1^\Delta \tau}.
\]

\[
(7.30)
\]

Also, to leading order in $\Delta \tau$, we approximate terms such as $\eta_1^\dagger \eta_0 \Delta \tau$ by $\eta_0^\dagger \eta_0 \Delta \tau$. If we take the limit and impose the $\eta_\beta = -\eta_0$ on the last matrix element to the left, we can rewrite the partition function as

\[
Z = \int \mathcal{D}\eta \int \mathcal{D}\eta \exp (-S)
\]

\[
(7.31)
\]

where, by analogy with the Lagrangian formalism, we define the following quantity

\[
S = \int_0^\beta d\tau \left( \eta^\dagger (\tau) \frac{\partial}{\partial \tau} \eta (\tau) + \epsilon (\tau) \eta^\dagger (\tau) \eta (\tau) \right)
\]

\[
(7.32)
\]

as the action $S$. We have generalized also to a time-dependent Hamiltonian. The integrand is like a Lagrangian when $\eta^\dagger (\tau)$ and $\eta (\tau)$ are taken as conjugate variables.

Thinking of the $\eta$ at different times as different variables, we can use our formula for Gaussian integrals over Grassmann variables Eq. (7.14) the partition function can be written as

\[
Z = \det \left( \frac{\partial}{\partial \tau} + \epsilon (\tau) \right) = \exp \left[ \text{Tr} \log \left( \frac{\partial}{\partial \tau} + \epsilon (\tau) \right) \right].
\]

\[
(7.33)
\]
The matrix entering determinant and trace above is defined by returning to the discrete representation.

In the case of a time-independent Hamiltonian, the determinant can be evaluated as follows. Go to the basis where the time derivative is diagonal, namely the Matsubara-frequency basis. Then, we obtain

\[
Z = \exp \left[ \text{Tr} \log \left( -i\omega_n + \varepsilon \right) \right] = \exp \left[ \sum_n \log \left( -i\omega_n + \varepsilon \right) e^{-i\omega_n,0^-} \right].
\] (7.34)

The factor \( e^{-i\omega_n,0^-} \) is made necessary to have a unique result. To verify that this formula is correct, we can use the expression for the occupation number

\[
n = \frac{\text{Tr} \left( \exp \left( -\beta H \right) c^\dagger c \right)}{\text{Tr} \left( \exp \left( -\beta H \right) \right)} = -\frac{\partial \ln Z}{\partial (\beta \varepsilon)} = T \sum_n e^{-i\omega_n,0^-} \frac{1}{1 + e^{\beta \varepsilon}}. \] (7.35)

Integrating, we recover the formula obtained in the canonical formalism Eq.(7.24).

To find the Green’s function or any higher order Green’s function, we add source fields and use derivatives. We can confirm that this works at the level of the Green’s function by starting from our previous result for Gaussian Grassmann integrals with sources, Eq.(7.18). We just rename the matrix \( A \) as \( -\hat{G}^{-1} \) and check that this is consistent with the definition of the Green’s function

\[
Z = \int \mathcal{D}\psi^\dagger \int \mathcal{D}\psi \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta \exp \left[ -S \right]
\]

\[
G (i\omega_n) = \frac{1}{Z} \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta \exp \left[ -\sum_n \eta^\dagger \left( -\hat{G}^{-1} \right) \eta \right] \mathcal{D}\eta^\dagger \mathcal{D}\eta
\]

\[
= -\frac{\partial^2 \ln Z}{\partial J^\dagger \partial J} \bigg|_{J=0} = -\frac{\partial^2 \ln \left[ \det \left( -\hat{G}^{-1} \right) \right] \exp \left( \mathbf{J}^\dagger \left( -\hat{G}^{-1} \right)^{-1} \mathbf{J} \right)}{\partial \mathbf{J}^\dagger \partial \mathbf{J}} \bigg|_{J=0} - \frac{\partial^2 \left( \mathbf{J}^\dagger \left( -\hat{G}^{-1} \right)^{-1} \mathbf{J} \right)}{\partial \mathbf{J}^\dagger \partial \mathbf{J}} \bigg|_{J=0}. \] (7.37)

7.1.6 Quantum impurities

Assume I have a single level with some Hubbard interaction and hybridization to a bath of non-interacting electrons. This time we restore spins. Let \( \psi_\sigma \) be the Grassman variables associated with the impurity, and \( \eta_\sigma (k) \) those associated with the bath. The levels in the bath are labeled by \( k \). The partition function then is

\[
Z = \int \mathcal{D}\psi^\dagger \int \mathcal{D}\psi \int \mathcal{D}\eta^\dagger \int \mathcal{D}\eta \exp \left[ -S \right]
\]

with

\[
S = S_I + S_{Ib} + S_b \] (7.40)
where the impurity action is

\[
S_I = \int_0^\beta d\tau \left[ \sum_\sigma \left( \psi_\sigma^\dagger (\tau) \frac{\partial}{\partial \tau} \psi_\sigma (\tau) + \varepsilon I \psi_\sigma^\dagger (\tau) \psi_\sigma (\tau) \right) + U \psi_1^\dagger (\tau) \psi_1 (\tau) \psi_1^\dagger (\tau) \psi_1 (\tau) \right] \]

(7.41)

with the bath

\[
S_b = \int_0^\beta d\tau \sum_k \sum_\sigma \left[ \eta_\sigma^\dagger (k, \tau) \frac{\partial}{\partial \tau} \eta_\sigma (k, \tau) + \varepsilon (k) \eta_\sigma^\dagger (k, \tau) \eta_\sigma (k, \tau) \right] \]

(7.42)

\[
= \int_0^\beta d\tau \sum_k \sum_\sigma \eta_\sigma^\dagger (k, \tau) \left( - G_b^{-1} (k, \tau) \right) \eta_\sigma (k, \tau)
\]

(7.43)

and the hybridization between impurity and bath

\[
S_{Ib} = \int_0^\beta d\tau \sum_k \sum_\sigma \left[ V_\sigma^* (k) \psi_\sigma^\dagger (\tau) \eta_\sigma (k, \tau) + V_\sigma (k) \eta_\sigma^\dagger (k, \tau) \psi_\sigma (\tau) \right].
\]

(7.44)

The functional integral over the bath degrees of freedom \( \eta_\sigma^\dagger (k, \tau) \), \( \eta_\sigma (k, \tau) \) can be done easily if we identify the source fields in the Gaussian Grassmann integral Eq.(7.18) as

\[
J_\sigma (k, \tau) = V_\sigma (k) \psi_\sigma (\tau).
\]

(7.45)

The integral over the bath degrees of freedom leaves us with

\[
Z = \exp \left[ \text{Tr} \log \left( G_b^{-1} \right) \right] \int \mathcal{D} \psi^\dagger \int \mathcal{D} \psi \exp \left[ - S_I + J^\dagger \left( - G_b^{-1} \right)^{-1} J \right].
\]

(7.46)

The prefactor is the determinant associated with the bath. It will drop out from observables associated only with the impurity. In Matsubara frequencies the bath Green’s function is diagonal so it is easy to rewrite the term involving the source as

\[
J^\dagger \left( - G_b \right) J = \sum_n \sum_\sigma \psi_\sigma^\dagger (i \omega_n) \left( \sum_k V_\sigma^* (k) \frac{1}{i \omega_n - \varepsilon (k)} V_\sigma (k) \right) \psi_\sigma (i \omega_n).
\]

(7.47)

This term thus just modifies \( G_0^{-1} \) in the impurity action. We define the hybridization function

\[
\Delta (i \omega_n) \equiv \sum_k V_\sigma^* (k) \frac{1}{i \omega_n - \varepsilon (k)} V_\sigma (k).
\]

(7.48)