6 Functional Integral for the Quantum Partition Function

We will make use of the coherent state formalism developed earlier to build the partition function as a functional integral. The quantum partition function is

$$\begin{aligned} Z &= \mathrm{Tr}\left[\mathrm{e}^{-\beta(\mathrm{H}-\mu\mathrm{N})}\right] \\ &= \sum_\alpha \langle\alpha|e^{-\beta(H-\mu N)}|\alpha\rangle \ , \end{aligned} \tag{6.1}$$

The identity in Fock space is given by

$$\int d\left(\bar{\phi},\phi\right)\ e^{-\sum_k \bar{\phi}_k\phi_k}\,|\phi\rangle\langle\phi| = \mathbb{1}_{\mathcal{F}} \ , \tag{6.2}$$

where $|\phi\rangle$ is a coherent state and we defined

$$d\left(\bar{\phi},\phi\right) \equiv \prod_i \frac{d\bar{\phi}_i, d\phi_i}{\pi} \ . \tag{6.3}$$

Inserting (6.2) in (6.1) we obtain

$$Z = \int d\left(\bar{\phi},\phi\right)\ e^{-\sum_k \bar{\phi}_k\phi_k} \sum_\alpha \langle\alpha|\phi\rangle\langle\phi|e^{-\beta(H-\mu N)}|\alpha\rangle \ . \tag{6.4}$$

Making use of the completeness relation

$$\sum_\alpha |\alpha\rangle\langle|\alpha| = 1 \ , \tag{6.5}$$

and assuming that the states $|\alpha\rangle$ are bosonic (so that we can switch $\langle\alpha|$ and $|\alpha\rangle$, if fermionic we pick up a minus sign in the process), we obtain

$$Z = \int d\left(\bar{\phi},\phi\right)\ e^{-\sum_k \bar{\phi}_k\phi_k}\langle\phi|e^{-\beta(H-\mu N)}|\phi\rangle \ . \tag{6.6}$$

The expression above looks similar to what we started with when we derived the Feynman path integral formulation of quantum mechanics. The are two differences: the time interval Δt is here $i\beta$, and the initial state is the same as the final state since the partition function is a trace. We will then proceed to define the functional integral where the integration functions are all the possible functional values that the ϕ_i's and $\bar{\phi}_i$'s can take. We then consider β the time interval and discretize it dividing it in M segments of length $\Delta\tau$ such that

$$\beta = M \times \Delta\tau \ , \tag{6.7}$$

as shown in Figure 6.1 below.

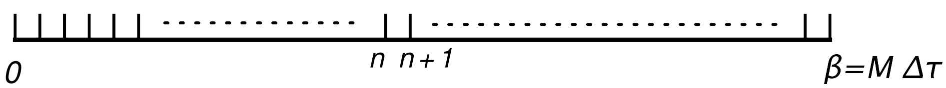

Figure 6.1: Discretization of β as a time interval, in discrete bits of size $\Delta\tau$.

The disretization then proceeds analogously to the case of quantum mechanics propagation amplitude. We have

$$\langle\phi_0|e^{-\Delta\tau(H-\mu N)}e^{-\Delta\tau(H-\mu N)}\ldots e^{-\Delta\tau(H-\mu N)}e^{-\Delta\tau(H-\mu N)}\ldots e^{-\Delta\tau(H-\mu N)}|\phi_M\rangle \ , \tag{6.8}$$

and now we insert the resolution of the identity in Fock space (6.2) in between each exponential in (6.8).

$$\langle\phi^0|e^{-\Delta\tau(H-\mu N)}|\phi^1\rangle\langle\phi^1|e^{-\Delta\tau(H-\mu N)}|\phi^2\rangle\ldots\langle\phi^n|e^{-\Delta\tau(H-\mu N)}|\phi^{n+1}\rangle\ldots e^{-\Delta\tau(H-\mu N)}|\phi^M\rangle \ , \tag{6.9}$$

where the integrals $\int d\left(\bar{\phi}^n, \phi^n\right)$ are understood. In particular, in the insertion between $|\phi^n\rangle$ and $|\phi^{n+1}\rangle$, we need to compute

$$I_n \equiv \int d\left(\bar{\phi}^n, \phi^n\right) e^{-\sum_k \bar{\phi}^n_k \phi^n_k}\langle\phi^n|e^{-\Delta\tau(H-\mu N)}|\phi^{n+1}\rangle \ , \tag{6.10}$$

Next, we need to act with H and N on the coherent states $|\phi^n\rangle$. But since they can be written in second quantization as

$$H = \sum_{i,j} h_{ij} a^\dagger_i a_j + \sum_{i,j,k,\ell} V_{ijk\ell} a^\dagger_i a^\dagger_j a_k a_\ell \ , \tag{6.11}$$

as well as the number of particles

$$N = \sum_i a_i^\dagger a_i \ . \tag{6.12}$$

Using that

$$a_i|\phi^n\rangle = \phi_i^n|\phi^n\rangle \ , \qquad \langle\phi^n|a_i^\dagger = \langle\phi^n|\bar{\phi}_i^n \ , \tag{6.13}$$

For instance, we have

$$\langle\phi^n|e^{-\Delta\tau\sum_{i,j} h_{ij} a_i^\dagger a_j}|\phi^{n+1}\rangle = e^{-\Delta\tau\sum_{i,j} h_{ij}\bar{\phi}_i^n\phi_j^{n+1}}\langle\phi^n|\phi^{n+1}\rangle \ , \tag{6.14}$$

and similarly for the interaction term and for N. On the other hand, we know that the product of coherent states satisfies

$$\langle\phi^n|\phi^{n+1}\rangle = e^{\sum_k \bar{\phi}_k^n\phi_k^{n+1}} \ . \tag{6.15}$$

Using the definition

$$\bar{\phi}^n\phi^{n+1} \equiv \sum_k \bar{\phi}_k^n\phi_k^{n+1} \ , \tag{6.16}$$

to simplify the notation, we arrive at

$$I_n = \int d\left(\bar{\phi}^n, \phi^n\right)\ e^{-\Delta\tau\left(\frac{(\bar{\phi}^n\phi^n - \bar{\phi}^n\phi^{n+1})}{\Delta\tau} + H(\bar{\phi}^n,\phi^{n+1}) - \mu N(\bar{\phi}^n,\phi^{n+1})\right)} \ , \tag{6.17}$$

where, for instance, we have

$$N(\bar{\phi}^n, \phi^{n+1}) = \sum_k \bar{\phi}_k^n\phi_k^{n+1} \ , \tag{6.18}$$

coming from evaluating

$$\langle\phi^n|e^{N(a_k^\dagger, a_k)}|\phi^{n+1}\rangle \ , \tag{6.19}$$

and similarly for $H(\bar{\phi}^n, \phi^{n+1})$. The partition unction is then obtained in the limit for $M \to \infty$ and $\Delta\tau \to 0$. This is

$$Z = \lim_{M\to\infty, \Delta\tau\to 0} \int \left(\prod_{n=1}^{M} d\left(\bar{\phi}^n, \phi^n\right) \right) e^{-S[\bar{\phi},\phi]} \ , \tag{6.20}$$

where we defined

$$S[\bar{\phi},\phi] = \sum_{n=1}^{M} \Delta\tau \left(\frac{(\bar{\phi}^n\phi^n - \bar{\phi}^n\phi^{n+1})}{\Delta\tau} + H(\bar{\phi}^n, \phi^{n+1}) - \mu N(\bar{\phi}^n, \phi^{n+1}) \right) . \tag{6.21}$$

This action defined above has the continuum limit

$$S[\bar{\phi},\phi] = \int_0^\beta d\tau \left\{ \bar{\phi}\partial_\tau\phi + H(\bar{\phi},\phi) - \mu N(\bar{\phi},\phi) \right\} \ , \tag{6.22}$$

where it is understood that the fields ϕ and $\bar{\phi}$ are functions of τ, i.e $\phi(\tau)$ and $\bar{\phi}(\tau)$. Then, the quantum partition function is written as a functional integral in the coherent state representation as

$$Z = \int \mathcal{D}(\bar{\phi})\mathcal{D}(\phi) e^{-S[\bar{\phi},\phi]} \ . \tag{6.23}$$

As usual, the measure of the function integral in (6.23) is

$$\mathcal{D}(\bar{\phi})\mathcal{D}(\phi) = \lim_{M\to\infty} \prod_{n=1}^{M} d\left(\bar{\phi}^n, \phi^n\right) \ . \tag{6.24}$$

Finally, since the partition function is a trace the integration over τ in (6.22) assumes the periodic (anti-periodic in the case of fermions) boundary conditions

$$\phi(0) = \phi(\beta) \ , \qquad \bar{\phi}(0) = \bar{\phi}(\beta) \ . \tag{6.25}$$

We have succeeded in writing the partition function as a functional integral in (6.23). We see that the integration is over all the possible functional forms of the ϕ and $\bar{\phi}$ eigenvalues of the coherent states. These are the fields in this formulation. Although we have exemplify every step for the case of bosons, i.e. commuting a_i and $a_i^\dagger$ operators, everything we have said can be rederived for fermions. The anti-commuting properties of the annihilation and creation operators are inherited by the fermionic fields, resulting in Grasmann variables in the functional integral. As mentioned earlier, the boundary conditions (6.25) in this case will be anti-periodic.

6.1 Frequency (Matsubara) Representation

Given the boundary conditions in (6.25), results in a discrete Fourier transform to the conjugate variable which we call ω_n given by

$$\phi(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \phi_n e^{-i\omega_n \tau} \ , \tag{6.26}$$

where we interpret the conjugate variables ω_n as frequencies, in the same sense τ is a time. The ϕ_n are the fields in the frequency or Matsubara representation. The inversion of (6.26) is

$$\phi_n = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau \, \phi(\tau) e^{i\omega_n \tau} \ . \tag{6.27}$$

The Matsubara frequencies take discrete values according with

$$\omega_n = \frac{2\pi n}{\beta}, \tag{6.28}$$

with n integer. They satisfy

$$\int_0^\beta d\tau \, e^{-i\omega_n \tau} = \delta_{0,n} \ . \tag{6.29}$$

For instance, if we consider the hamiltonian in (6.11), the action (6.22) can be expressed in the Matsubara representation as

$$S[\bar{\phi}, \phi] = \sum_{i,j,n} \bar{\phi}_{in} \left[(-i\omega_n - \mu) \, \delta_{ij} + h_{ij} \right] \phi_{jn} + \frac{1}{\beta} \sum_{i,j,k,\ell,n_i} V_{ijk\ell} \bar{\phi}_{in_1} \bar{\phi}_{jn_2} \phi_{kn_3} \phi_{\ell n_4} \delta_{n_1+n_2, n_3+n_4} \ , \tag{6.30}$$

where we used (6.29).

6.2 Free Electron Gas

As a simple application fo the Matsubara representation we consider the example of a free electron gas. Then the hamiltonian can be written as

$$
\begin{aligned}
H &= H_0(\bar{\phi},\phi) = \sum_{i,j} H_{0ij}\bar{\phi}_i\phi_j \\
&= \sum_a \epsilon_a \bar{\phi}_a(\tau)\phi_a(\tau) \ ,
\end{aligned} \tag{6.31}
$$

where in the last line we used the fact that we can always diagonalize H_0, and ϵ_a are the eigenvalues. Then, in the Matsubara representation we have

$$
S[\bar{\phi},\phi] = \sum_a \sum_n \bar{\phi}_{an} \left(-i\omega_n + \epsilon_a - \mu\right) \phi_{an} \ , \tag{6.32}
$$

Then the functional integral can be factorized as

$$
Z = \int \prod_a \left[\mathcal{D}(\bar{\phi}_a)\mathcal{D}(\phi_a) e^{-\sum_n \bar{\phi}_a(-i\omega_n+\xi_a)\phi_a} \right] \equiv \prod_a Z_a \ , \tag{6.33}
$$

where we defined $\xi_a = \epsilon_a - \mu$ and

$$
\begin{aligned}
Z_a &= \int \mathcal{D}(\bar{\phi}_a)\mathcal{D}(\phi_a) e^{-\sum_n \bar{\phi}_a(-i\omega_n+\xi_a)\phi_a} \\
&= \prod_n \left[\beta\left(-i\omega_n + \xi_a\right)\right]^{-1} \\
&= \det\left[\beta\left(-i\hat{\omega} + \xi_a\right)\right]^{-1} \ ,
\end{aligned} \tag{6.34}
$$

where the factor of β in the last two lines appears as a consequence of changing the integration variables from ϕ's in the τ representation to the ones in the Matsubara formalism, the -1 exponent corresponds to the boson case and should be replace with a $+1$ for fermions, and we defined the operator $\hat{\omega}$ by

$$
\hat{\omega}_{n,n'} = \omega_n \, \delta_{n,n'} \ . \tag{6.35}
$$

We could use this partition function to compute the distribution of bosons or fermions. This would require to perform sums over the Matsubara frequencies. Although this looks too complicated to obtain such a simple result, the advantage of the field theory formulation appears in more complex situations.

Additional suggested readings

- *Condensed Matter Field Theory*, Altland and Simons, Section 4.2.
- *Quantum Theory of Many Particle Systems*, A. L. Fetter and J. D. Walecka, Chapters 1 and 2.