4.2 Field integral for the quantum partition function

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

Introduce a resolution of identity using coherent ~~states~~

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

↑ c.s. notes

To do: get rid of $\sum_n$.

ζ: $+1$ B, -1 F

Use fact ~~that~~ $\langle n|\psi\rangle\langle\psi|n\rangle = \langle \zeta\psi|n\rangle\langle n|\psi\rangle$

Why? F: use $|n\rangle = a^\dagger_{i_1}\cdots a^\dagger_{i_m}|0\rangle$ $\quad \langle n| = \langle 0|a_{i_m}\cdots a_{i_1}$

$$\langle n|\psi\rangle = \langle 0|a_{i_m}\cdots a_{i_1}|\psi\rangle = \langle 0|\psi_{i_m}\cdots\psi_{i_1}|\psi\rangle = \psi_{i_m}\cdots\psi_{i_1}\underbrace{\langle 0|\psi\rangle}_{1}$$

$$\langle\psi|n\rangle = \ldots = \bar{\psi}_{i_1}\cdots\bar{\psi}_{i_m}$$

Thus: $\langle n|\psi\rangle\langle\psi|n\rangle = \psi_{i_m}\cdots\psi_{i_1}\bar\psi_{i_1}\cdots\bar\psi_{i_m}$

$$= \underbrace{\psi_{i_1}\bar\psi_{i_1}}_{\zeta\bar\psi_{i_1}\psi_{i_1}}\psi_{i_2}\bar\psi_{i_2}\cdots\psi_{i_m}\bar\psi_{i_m} = \underbrace{(\zeta\bar\psi_{i_1})\cdots(\zeta\bar\psi_{i_m})}_{\langle\zeta\psi|n\rangle}\underbrace{\psi_{i_m}\cdots\psi_{i_1}}_{\langle n|\psi\rangle}$$

$$= (\zeta\bar\psi_{i_1}\psi_{i_1})(\zeta\bar\psi_{i_2}\psi_{i_2})\cdots(\zeta\bar\psi_{i_m}\psi_{i_m}) =$$

Therefore our partition fn is

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

& use $\sum_n |n\rangle\langle n| = \mathbb{1}$

In consequence,

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

Assume that our Hamiltonian is in normal-ordered form

$$\hat{H}(a^\dagger, a) = \sum_{ij} h_{ij}\, a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l$$

FPI: $e^{-\frac{i}{\hbar}\hat{H}t}$ split time interval t in N ~~steps~~ steps of $\Delta t = \frac{t}{N}$

$N \to \infty$

Here: $e^{-\beta(\hat{H}-\mu\hat{N})}$ split "imaginary" time β in N steps

$$= \prod_{n=1}^{N} e^{-\frac{\beta}{N}(\hat{H}-\mu\hat{N})} \qquad \int d(\bar{\psi}^n, \psi^n)\, e^{-\sum_i \bar{\psi}_i^n \psi_i^n} |\psi^n\rangle\langle\psi^n|$$

Thus:

$$Z = \int d(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i \psi_i} \langle \zeta\psi |\, \underbrace{e^{-\frac{\beta}{N}(\hat{H}-\mu\hat{N})}\, \mathbb{1}_{N-1} \cdots \mathbb{1}_{n+1} e^{\cdots}\, \mathbb{1}_n e^{\cdots} \cdots \mathbb{1}_1\, e^{-\frac{\beta}{N}(\hat{H}-\mu\hat{N})}}_{N \text{ times}} |\psi\rangle$$

Needed:

$$\langle \psi_{n+1} | e^{-\frac{\beta}{N}(\hat{H}-\mu\hat{N})} | \psi_n \rangle = \langle \psi_{n+1} | \left\{ 1 - \frac{\beta}{N}(\hat{H}-\mu\hat{N}) + O\left(\frac{1}{N^2}\right) \right\} | \psi_n \rangle$$

$$= \left\{ 1 - \delta\, H(\bar{\psi}^{n+1}, \psi^n) - \mu N(\ldots) \right\} \langle \psi_{n+1} | \psi_n \rangle = e^{-\delta(H-\mu N)} \langle \psi^{n+1} | \psi^n \rangle$$

Because $\hat{H}$ is normal ordered, we have

$$\langle \psi_{n+1} | \hat{H}(a^\dagger, a) | \psi_n \rangle = \langle \psi_{n+1} | H(\bar{\psi}_{n+1}, \psi_n) | \psi_n \rangle$$

$$= H(\bar{\psi}_{n+1}, \psi_n) \langle \psi_{n+1} | \psi_n \rangle$$

For example, $\hat{H}(a^\dagger, a) = a_1^\dagger a_2 + a_1^\dagger a_2^\dagger a_3 a_4$

Then, $$\langle \psi_{n+1} | \hat{H} | \psi_n \rangle = \left(\bar{\psi}_1 \psi_2 + \bar{\psi}_1 \bar{\psi}_2 \psi_3 \psi_4 \right) \underbrace{\langle \psi_{n+1} | \psi_n \rangle}_{e^{\sum_i \bar{\psi}_i^{n+1} \psi_i^n}}$$

Done,

$$Z = \int \prod_{n=0}^{N-1} d(\bar{\psi}^n, \psi^n)\, e^{-\sum_{n=0}^{N-1} \bar{\psi}_i^n \psi_i^n} \langle \psi^N = \zeta \psi^0 | e^{-\overset{\beta/N}{\delta}(H - \mu N)} | \psi^{N-1} \rangle \langle \psi^{N-1} | \dots | \psi^0 \rangle$$

$$= \int_{\substack{\bar{\psi}^N = \zeta \bar{\psi}^0 \\ \psi^N = \zeta \psi^0}} \prod_{n=0}^{N-1} d(\bar{\psi}^n, \psi^n) \exp\left\{ -\sum_{n=0}^{N-1} \sum_i \left[\bar{\psi}_i^n - \bar{\psi}_i^{n+1} \right] \psi_i^n - \delta \sum_{n=0}^{N-1} \left[H(\bar{\psi}^{n+1}, \psi^n) - \mu N(\bar{\psi}^{n+1}, \psi^n) \right] \right\}$$

Cleaner notation: define $\partial_\tau \bar\psi \equiv \frac{\bar\psi^{n+1} - \bar\psi^{n}}{\delta}$

& $\mathcal{D}(\bar\psi, \psi) = \lim_{N \to \infty} \prod_{n=0}^{N-1} d(\bar\psi^n, \psi^n)$

to get

$$\boxed{Z = \int \mathcal{D}(\bar\psi, \psi)\, e^{-S[\bar\psi, \psi]} \Big|_{\substack{\bar\psi(\beta) = \zeta\bar\psi(0) \\ \psi(\beta) = \zeta\psi(0)}} \qquad S[\bar\psi, \psi] = \int_0^\beta d\tau \left[\sum_i \bar\psi_i(\tau)\partial_\tau \psi_i(\tau) + H(\bar\psi(\tau), \psi(\tau)) - \mu N(\bar\psi(\tau), \psi(\tau)) \right]}$$

Because fields obey $\psi(\beta) = \xi\,\psi(0)$ (& same for $\bar\psi$), it's convenient to Fourier transform them.

Matsubara repres$^{\underline{n}}$:

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \psi_n e^{-i\omega_n \tau} \qquad \psi_n = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\, \psi(\tau) e^{i\omega_n \tau}$$

$$\bar\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \bar\psi_n e^{i\omega_n \tau} \qquad \bar\psi_n = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\, \bar\psi(\tau) e^{-i\omega_n \tau}$$

$$\omega_n = \begin{cases} \frac{2\pi}{\beta} n & \text{bosons} \\ \frac{2\pi}{\beta}(n+\frac{1}{2}) & \text{fermions} \end{cases}$$

Using ~~this~~ Randy Matsubara repres^{n}, we get our final & favourite version

$$Z = \int \mathcal{D}(\overline{\psi},\psi)\, e^{-S[\overline{\psi},\psi]} \qquad \mathcal{D}(\overline{\psi},\psi) = \prod_{n} d(\overline{\psi}_n,\psi_n)$$

n = Matsubara indices

For $H = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l$, ~~then~~

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

n = Matsubara

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

where we used $\int_0^\beta d\tau\, e^{-i(\omega_m - \omega_n)\tau} = \beta\,\delta_{n,m}$

Example of the noninteracting gas

$$H = \sum_i \varepsilon_i a_i^\dagger a_i \qquad \xi_i \equiv \varepsilon_i - \mu$$

Effective action: $$S = \sum_i \sum_n \bar{\phi}_{in} \left(-i\omega_n + \xi_i \right) \phi_{in} \equiv \sum_i S_i$$

Partition fn: $$Z = \int \mathcal{D}(\bar{\phi},\phi)\, e^{-S[\bar{\phi},\phi]} = \prod_i Z_i$$

$$Z_i = \int \mathcal{D}(\bar{\phi}_i,\phi_i)\, e^{-S_i}$$

$$= \int \left[\prod_n d(\bar{\phi}_n,\phi_n) \right] e^{-\sum_n \bar{\phi}_n (-i\omega_n + \xi_i) \phi_n} = \prod_n \left[\int d(\bar{\phi}_n,\phi_n)\, e^{-\bar{\phi}_n(-i\omega_n + \xi_i)\phi_n} \right]$$

Using the measure def: $$d(\bar{\phi}_n,\phi_n) = \begin{cases} \frac{1}{\pi\beta}\, d\bar{\phi}_n\, d\phi_n & \text{Bosons} \\ \beta\, d\bar{\phi}_n\, d\phi_n & \text{Fermions} \end{cases}$$

such that $$\int d(\bar{\phi}_n,\phi_n)\, e^{-\bar{\phi}_n \varepsilon \phi_n} = (\beta\varepsilon)^{-\zeta}$$

Performing the integrals, we get

$$Z = \prod_i \prod_n \left[\beta(-i\omega_n + \xi_i)\right]^{-\zeta}$$

Free energy $\quad F = -T \ln Z = T\zeta \sum_i \sum_n \ln\left[\beta(-i\omega_n + \xi_i)\right]$

The bad news: need to perform $\sum_n$ (some f^{ns} of ω_n)

The good news: Cauchy's theorem

See notes for general theory of Matsubara summations.

Here, need result in eq^{n} (4.80)

$$\Rightarrow \quad F = T\zeta \sum_i \ln\left[1 - \zeta e^{-\beta \xi_i}\right]$$