PARTITION FUNCTION

$$Z = \int \mathcal{D}[\vec{\bar{\psi}}(\tau), \vec{\psi}(\tau)]\, e^{-S_E[\bar{\psi},\psi]} = \mathrm{tr}\, e^{-\beta(H-\mu N)}$$

$$S_E = \int_0^\beta d\tau\ \vec{\bar{\psi}} \cdot \left(\frac{\partial}{\partial\tau} - \mu\right)\vec{\psi} + H[\vec{\bar{\psi}},\psi]$$

WITH $\begin{cases} \vec{\psi}(0) = \zeta\vec{\psi}(\beta) \\ \vec{\bar{\psi}}(0) = \zeta\vec{\bar{\psi}}(\beta) \end{cases}$ $\boxed{\text{BOUNDARY CONDITIONS}}$

$[S_E] = 1, \quad [\tau] = (\text{ENERGY})^{-1}$

(IN UNITS WHERE $\hbar = 1$)

MORE EXPLICITLY, FOR $H = \sum_{i,j} a_i^+ h_{ij} a_j + \sum_{ijkl} a_i^+ a_j^+ V_{ijkl} a_l a_k$

$$S_E = \int_0^\beta d\tau \left\{ \sum_{i,j} \bar{\psi}_i(\tau)\left[\left(\frac{\partial}{\partial\tau} - \mu\right)\delta_{ij} + h_{ij}\right]\psi_j(\tau) + \sum_{i,j,k,l} V_{ijkl}\ \bar{\psi}_i(\tau)\bar{\psi}_j(\tau)\psi_l(\tau)\psi_k(\tau) \right\}$$

- MATSUBARA FREQUENCIES

DUE TO PERIODICITY, FOURIER TRANSFORM

DEFINITION $\begin{cases} \vec{\psi}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \vec{\psi}_n e^{-i\omega_n\tau} \\ \vec{\bar{\psi}}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \vec{\bar{\psi}}_n e^{i\omega_n\tau} \end{cases}$

INVERSE $\vec{\psi}_n = \frac{1}{\sqrt{\beta}} \int_0^\beta d\tau\ \vec{\psi}(\tau)\, e^{i\omega_n\tau}$

WHERE $\cancel{\omega_m}$ $e^{i\omega_m \beta} = \xi$ ②

$$\Rightarrow \omega_m = \begin{cases} \frac{2\pi}{\beta} m = 2\pi m T , & \text{FOR BOSONS } (\xi = 1) \\ \frac{\pi}{\beta}(2m+1) = (2m+1)\pi T , & \text{FOR FERMIONS } (\xi = -1) \end{cases}$$

(IN UNITS WHERE $k_B = 1$) $[\omega_m] = \text{ENERGY}$

THUS,

$$S_E = \sum_{i,j,m,n} \bar{\psi}_{i,m} \left[(-i\omega_m - \mu)\delta_{ij} + h_{ij} \right] \psi_{j,n} \int_0^\beta \frac{e^{-i(\omega_m - \omega_n)\tau}}{\beta} d\tau$$

$$+ \sum_{ijkl} \sum_{\substack{m_1 m_2 \\ m_3 m_4}} \bar{\psi}_{i,m_1} \bar{\psi}_{j,m_2} V_{ijkl} \psi_{l m_3} \psi_{k m_4} \int_0^\beta d\tau \frac{e^{-i(\omega_{m_3} + \omega_{m_4} - \omega_{m_1} - \omega_{m_2})\tau}}{\beta^2}$$

$$\boxed{S_E = \sum_{i,j,m} \bar{\psi}_{i,m} \left[(-i\omega_m - \mu)\delta_{ij} + h_{ij} \right] \psi_{j,m} + \sum_{ijkl} \sum_{\substack{m_1 m_2 \\ m_3 m_4}} \bar{\psi}_{i m_1} \bar{\psi}_{j m_2} \frac{V_{ijkl}}{\beta} \psi_{l m_3} \psi_{k m_4} \delta_{m_1 + m_2 , m_3 + m_4}}$$

NON-INTERACTING CASE

③

$$H_0 = \sum_{i,j} \bar{\psi}_i h_{ij} \psi_j \xrightarrow[\text{TRANSFORMATION}]{\text{UNITARY}} \sum_i \epsilon_i \bar{\phi}_i \phi_i$$

$$\Rightarrow S_E = \sum_{j,m} \bar{\phi}_{j,m} \left(-i\omega_m + \varepsilon_j \right) \phi_{j,m} \quad , \quad \varepsilon_j = \epsilon_j - \mu$$

DECOUPLED (i,m) MODES

$$Z = \int D[\vec{\bar{\phi}}, \vec{\phi}]\, e^{-S_E} = \int D[\vec{\bar{\phi}}, \vec{\phi}]\, e^{-\bar{\phi}_{1,1}[\varepsilon_1 - i\omega_1]\phi_{1,1}}\, e^{-\bar{\phi}_{1,2}[\varepsilon_1 - i\omega_2]\phi_{1,2}} \cdots$$

$$= \prod_{j,m} \int d(\bar{\phi}, \phi)\, e^{-\bar{\phi}(\varepsilon_j - i\omega_m)\phi}$$

$$= \prod_{j,m} \left[\beta \left(\epsilon_j - \mu - i\omega_m \right) \right]^{-\zeta}$$

JACOBIAN WHEN CHANGING $\phi(\tau) \to \phi_m$

$$d(\bar{\phi}(\tau), \phi(\tau)) = \beta\, d\left(\frac{\bar{\phi}(\tau)}{\sqrt{\beta}}, \frac{\phi(\tau)}{\sqrt{\beta}} \right) = \beta\, d(\bar{\phi}_m, \phi_m)$$

$$\rightarrow d(\bar{\phi}_m, \phi_m)$$

- FREE ENERGY $\equiv F = -\frac{1}{\beta} \ln Z$
(GRAND POTENTIAL)

$$\boxed{F = \frac{\zeta}{\beta} \sum_{j,m} \ln\left(\beta(\epsilon_j - \mu - i\omega_m) \right)}$$

MATSUBARA FREQUENCY SUMMATION

WE WILL, IN MANY OCCASIONS, COMPUTE SUMS OVER THE MATSUBARA FREQUENCIES ω_m. THERE IS A GENERAL FRAMEWORK FOR SUCH.

LET $S = \sum_m h(\omega_m)$ BE A SUM OVER THE MATSUBARA FREQUENCIES ω_m

- INTRODUCE AN AUXILIARY FUNCTION $g(z)$ WITH POLES AT $z = i\omega_m$ WITH <u>CONVENIENT</u> RESIDUES

USUALLY, $g(z) = \dfrac{\zeta\beta}{e^{\beta z} - \zeta}$ [SOMETIMES, IT IS USED $g(z) = \frac{\zeta\beta}{2}\left(\coth\left(\frac{\beta z}{2}\right)\right)^{\zeta}$]

- POLES AT $e^{\beta z} = \zeta \Rightarrow z = i\omega_m \equiv i * \begin{pmatrix}\text{MATSUBARA}\\ \text{FREQUENCIES}\end{pmatrix}$

- RESIDUES ARE $\dfrac{\zeta\beta}{\frac{\partial}{\partial z}(e^{\beta z} - \zeta)\Big|_{z=i\omega_m}} = \dfrac{\zeta\beta}{\beta e^{i\omega_m\beta}} = \dfrac{\zeta\beta}{\beta\zeta} = \underset{\text{CONVENIENT RESIDUE}}{\underset{\downarrow}{1}}$

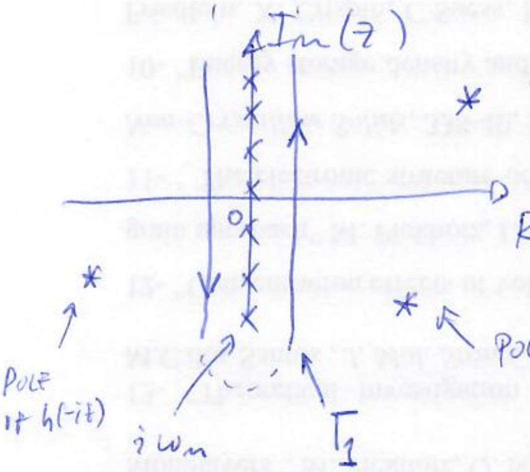
THEREFORE, $\dfrac{1}{2\pi i}\oint_{\Gamma_1} dz\, g(z)\, h(-iz) = \sum_{\substack{\text{RESIDUES}\\ \text{IN}\\ \Gamma_1}} g(z)\, h(-iz)\Big|_{z=z_N}$

CHOOSING Γ_1 CONTAINING ONLY THE RESIDUES OF g, i.e. THE $i\omega_m$, THEN, $z_m = i\omega_m$

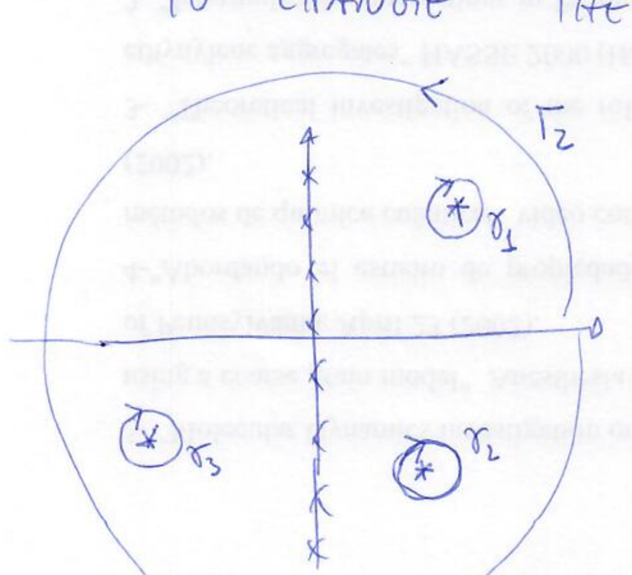
$$\rightarrow \sum_{\text{RESIDUES}} g(z)\, h(-iz)\Big|_{z=i\omega_n} = \sum_m h(\omega_m) = S$$

$$\rightarrow \boxed{S = \frac{1}{2\pi i}\oint_{\Gamma} dz\, g(z)\, h(-iz)}$$

THIS WORKS AS LONG AS THE POLES OF $h(-it)$ ARE NOT IN THE COMPLEX AXIS



• WHEN $g(z)\, h(-it) \rightarrow 0$ FASTER THAN $\frac{1}{|z|}$ FOR $|z| \rightarrow \infty$, IT IS USEFUL TO "CHANGE" THE INTEGRATION CONTOUR TO



$$S = \oint_{\Gamma_1} \cdots = \oint_{\Gamma_2} + \sum_k \oint_{\gamma_k}$$

$$\oint_{\Gamma_2} \cdots = 0 \qquad g(z)\, h(-iz) \rightarrow 0$$

$$\sum_k \oint_k = -\sum_{\substack{\text{RESIDUES}\\ \text{OF } h}} \text{Res}\big(g(z)\, h(-iz)\big)\Big|_{z=z_k}$$

EXAMPLE: $h(\omega_n) = \frac{1}{\zeta\beta}\frac{1}{\epsilon_j-\mu-i\omega_n}$

POLE @ $z = i\omega_n = \epsilon_j - \mu$

$$\Rightarrow S = \sum_n h(\omega_n) = -\mathrm{RES}\left(g(z)\,h(-iz)\right)\Big|_{z=\epsilon_j-\mu}$$

$$= \frac{-\zeta\beta}{e^{\beta(\epsilon_j-\mu)}-\zeta} * \frac{-1}{\zeta\beta} = \frac{1}{e^{\beta(\epsilon_j-\mu)}-\zeta} = \langle n_j\rangle$$

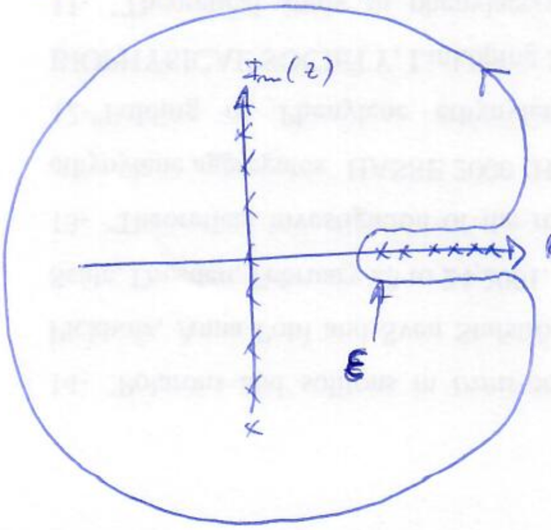
IN OTHER WORDS: $\boxed{\langle n_j\rangle = \frac{1}{\zeta\beta}\sum_n \frac{1}{\epsilon_j-\mu-i\omega_n}}$

BACK TO THE FREE ENERGY (GRAND POTENTIAL)

$$F = \frac{\zeta}{\beta}\sum_j\sum_n \ln\left(\beta(\epsilon_j-\mu-i\omega_n)\right)$$

$$\Rightarrow h(\omega_n) = \ln\beta(\epsilon - i\omega_n) \to h(-iz) = \ln(\epsilon-z)\beta$$

IN THIS CASE, WE HAVE A BRANCH CUT FOR $z>\epsilon$ IN THE REAL AXIS



$$\Rightarrow S = \sum_n h(\omega_n) = \frac{\oint_{\Gamma_2}^{\to 0} + \int_\infty^\epsilon (z=x-i0) + \int_\epsilon^\infty (z=x+i0)}{2\pi i}$$

$\boxed{\text{ENLARGE LIMITS!}}$

NOTICE THAT

$$\int_\infty^\epsilon (x-iy) + \int_\epsilon^\infty (x+iy) = \int_\infty^{-\infty}(x-iy) + \int_{-\infty}^\infty (x+iy),\quad y\to 0^+$$

BECAUSE $g(x-iy)\,h(-i(x-iy)) = g(x+iy)\,h(-i(x+iy))$ FOR $x<\epsilon$

THUS, $$S = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dx \; g(x)\left[\ln \beta(\varepsilon - x - i\eta) - \ln \beta(\varepsilon - x + i\eta)\right]$$

$$= \qquad \text{with} \quad g(x) = \frac{\zeta\beta}{e^{\beta x} - \zeta}\,, \quad \eta \to 0^+$$

INTEGRATION BY PARTS

$$g(x) = \frac{\partial}{\partial x}\ln\left(1 - \zeta e^{\beta x}\right)$$

$$\Rightarrow S = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} dx \; \ln\left(1 - \zeta e^{-\beta x}\right)\left(\frac{1}{x + i\eta - \varepsilon} - \frac{1}{x - i\eta - \varepsilon}\right)$$

$$= \frac{-1}{2\pi i}\int dx \; \ln\left(1 - \zeta e^{-\beta x}\right)\left(P\left(\frac{1}{x-\varepsilon}\right) - i\pi\,\delta(x-\varepsilon) - \left[P\left(\frac{1}{x-\varepsilon}\right) + i\pi\,\delta(x-\varepsilon)\right]\right)$$

$$= \int dx \; \ln\left(1 - \zeta e^{-\beta x}\right)\delta(x - \varepsilon)$$

$$\boxed{S = \ln\left(1 - \zeta e^{-\beta\varepsilon}\right)}$$

THUS, $$\boxed{F = \frac{\zeta}{\beta}\sum_j \ln\left(1 - \zeta e^{-\beta(\epsilon_j - \mu)}\right)}$$

$$\boxed{Z = e^{-\beta F} = \prod_j \left(1 - \zeta e^{-\beta(\epsilon_j - \mu)}\right)^{-\zeta}}$$

THIS IS THE WELL-KNOWN GRAND PARTITION FUNCTION OF NON-INTERACTING QUANTUM SYSTEMS

WHICH, IN THE NON-INTERACTING CASE, IS MUCH EASIER TO OBTAIN IN THE STANDARD QUANTUM STAT. MECH. FRAMEWORK.