A.2.a Matsubara formalism

- Basic idea: Use the formal analogy between the unnormalized thermal state operator $\tilde{\rho} = e^{-\beta H}$ and the time-evolution operator $U(t,0) = e^{-iHt}$.

- Introducing the time-like variable τ, $0 < \tau \leq \beta$, $\tilde{\rho}$ satisfies the equation: $\frac{\partial}{\partial \tau} \tilde{\rho}(\tau) = -H \tilde{\rho}(\tau)$, where $\tilde{\rho}(0) = \mathbb{1}$,

  and $\tilde{\rho}(\beta) = \tilde{\rho} = e^{-\beta H}$.

- By means of the Wick rotation $\boxed{t \leftrightarrow -i\tau}$ this maps to the standard Schrödinger equation.

- The analog of Heisenberg operators is given by Matsubara operators:

$$\Psi_H^M(x,\tau) = e^{H\tau}\Psi(x)e^{-H\tau}, \quad \overline{\Psi}_H^M(x,\tau) = e^{H\tau}\Psi^+(x)e^{-H\tau},$$

note that $\boxed{\overline{\Psi}_H^M \neq (\Psi_H^M)^+}$.

$$\rightsquigarrow \quad \frac{\partial}{\partial\tau}\Psi_H^M(x,\tau) = [H, \Psi_H^M(x,\tau)], \quad \frac{\partial}{\partial\tau}\overline{\Psi}_H^M(x,\tau) = [H, \overline{\Psi}_H^M(x,\tau)]$$

- The Matsubara Green's function is defined as

$$G_M(x,\tau;x',\tau') = -\left\langle T_M\left(\Psi_H^M(x,\tau)\overline{\Psi}_H^M(x',\tau')\right)\right\rangle =$$

$$= -\mathrm{Tr}\left\{\frac{e^{-\beta H}}{Z}T_M\left(\Psi_H^M(x,\tau)\overline{\Psi}_H^M(x',\tau')\right)\right\},$$

where the Matsubara time-ordering operator T_M is analogous to T, just for the thermal "time" variable τ.

- Periodicity of G_M in τ

spatial arguments dropped

- Due to the cyclic property of the trace, $G_M(\tau,\tau') = G_M(\tau-\tau')$
- $\tau-\tau' \in [-\beta,\beta] \rightsquigarrow G_M(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} G_M(\omega_n)\, e^{-i\omega_n\tau}$ with $\omega_n = \frac{\pi n}{\beta}$

Matsubara frequencies

- Choosing $\tau<0$, let us calculate $G_M(\tau)$ and $G_M(\tau+\beta)$:

$$G_M(\tau) = \underset{\text{Bosons}}{\overset{\text{Fermions}}{\pm}} \frac{1}{Z}\,\mathrm{Tr}\left\{e^{-\beta H}\psi^+ e^{H\tau}\psi e^{-H\tau}\right\} = \pm\frac{1}{Z}\,\mathrm{Tr}\left\{e^{-H(\beta+\tau)}\psi^+ e^{H\tau}\psi\right\}$$

$$G_M(\tau+\beta) \underset{\tau+\beta>0}{=} -\frac{1}{Z}\,\mathrm{Tr}\left\{e^{-\beta H} e^{H(\tau+\beta)}\psi e^{-H(\tau+\beta)}\psi^+\right\} = -\frac{1}{Z}\,\mathrm{Tr}\left\{e^{H\tau}\psi e^{-H(\tau+\beta)}\psi^+\right\}$$

$$\underset{\substack{\text{Cyclic}\\ \text{property}}}{=} -\frac{1}{Z}\,\mathrm{Tr}\left\{e^{-H(\tau+\beta)}\psi^+ e^{H\tau}\psi\right\} = \underset{\text{Bosons}}{\overset{\text{Fermions}}{\mp}} G_M(\tau).$$

$\rightsquigarrow$ $G_M(\tau)$ anti-periodic with β for fermions and periodic with β for bosons

$\hookrightarrow$ $$\boxed{\omega_n^F = \frac{(2n+1)\pi}{\beta} \quad ; \quad \omega_n^B = \frac{2n\pi}{\beta}}$$ Matsubara frequencies

- Diagrammatic perturbation theory for the Matsubara GF

- Matsubara interaction picture for $H = H_0 + V$:

$$\psi^M(x,\tau) = e^{H_0\tau}\psi(x)e^{-H_0\tau}, \quad S_M(\tau_1,\tau_2) = e^{H_0\tau_1}e^{-H(\tau_1-\tau_2)}e^{-H_0\tau_2}.$$

which satisfies $\frac{\partial}{\partial\tau_1}S_M(\tau_1,\tau_2) = -V^M(\tau_1)S_M(\tau_1,\tau_2)$;

with $V^M(\tau) = e^{H_0\tau}Ve^{-H_0\tau}$.

$$\rightsquigarrow \quad S_M(\tau_1,\tau_2) = J_M\, e^{-\int_{\tau_1}^{\tau_2} d\tau\, V^M(\tau)}$$

- By formal analogy to the Dirac interaction picture, we get:

$$G_M(x_1,\tau_1;x_2,\tau_2) = -\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H_0} J_M\left(S_M(\beta,0)\,\Psi^M(x_1,\tau_1)\,\overline{\Psi}^M(x_2,\tau_2)\right)\right) =$$

$$= -\frac{Z_0}{Z}\left\langle J_M\left(S_M(\beta,0)\,\Psi^M(x_1,\tau_1)\,\overline{\Psi}^M(x_2,\tau_2)\right)\right\rangle_0$$

with $\langle \ldots \sim \rangle_0 = \mathrm{Tr}\left(\frac{e^{-\beta H_0}}{Z_0}\ldots\ldots\right)$.

Using $\frac{Z_0}{Z} = \left(\frac{1}{Z_0}\mathrm{Tr}(e^{-\beta H})\right)^{-1} = \left(\langle e^{\beta H_0} e^{-\beta H}\rangle_0\right)^{-1} = \left(\langle S_M(\beta,0)\rangle_0\right)^{-1}$,

we get

$$\boxed{G_M(x_1,\tau_1;x_2,\tau_2) = -\frac{\left\langle J_M\left(S_M(\beta,0)\,\Psi^M(x_1,\tau_1)\,\overline{\Psi}^M(x_2,\tau_2)\right)\right\rangle_0}{\langle S_M(\beta,0)\rangle_0}}$$

- Since the cancellation theorem and Wick's theorem remain valid under the Wick rotation, the diagrammatic expansion is completely analogous to the $T=0$ case, by simply reinterpreting $\Leftarrow = -G_M$, $\leftarrow = -G_M^0$, $\bullet\!\!\dashrightarrow\!\!\bullet = -U$.

(note the absence of "i" prefactors)

- Practical complication: Rather than integrating frequency variables, we need to sum on discrete frequencies ω_n^F or ω_n^B in the Matsubara formalism.

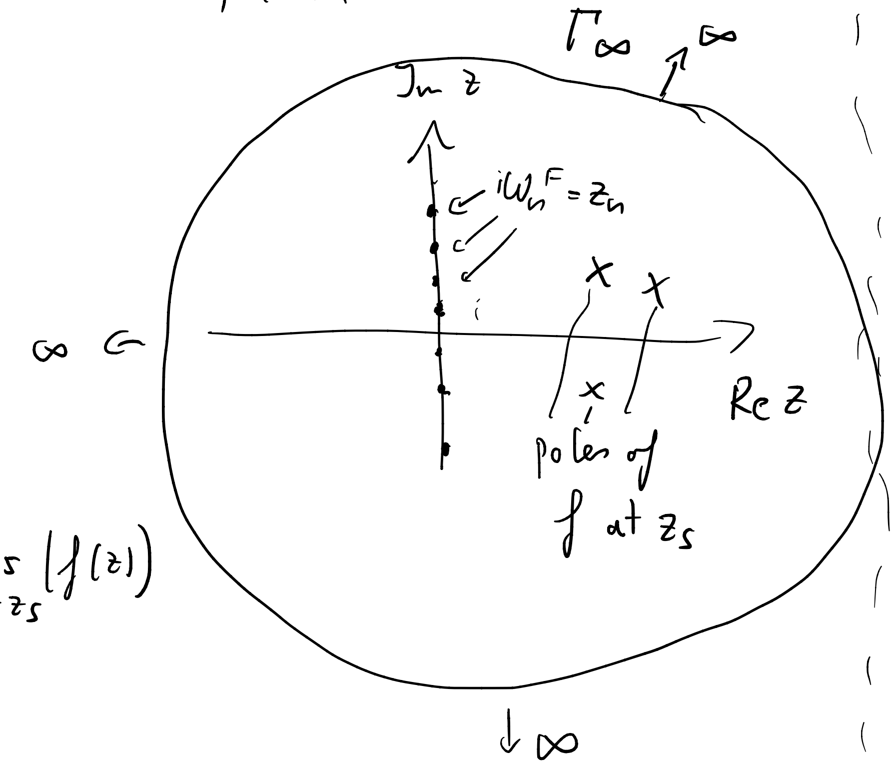
↳ useful trick: If $|f(z)| \leq |z|^{-(1+\varepsilon)}$ for $|z| \to \infty$ with $\varepsilon > 0$, we get:

$$\frac{1}{\beta} \sum_{n=-\infty}^{+\infty} f(i\omega_n^F) = -\frac{1}{2} \sum_s \left[\tanh\left(\frac{\beta z_s}{2}\right) \operatorname*{Res}_{z=z_s} f(z) \right] ; \quad \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} f(i\omega_n^B) = -\frac{1}{2} \sum_s \left[\coth\left(\frac{\beta z_s}{2}\right) \operatorname*{Res}_{z=z_s} (f(z)) \right]$$

as $\tanh \frac{\beta z}{2}$ $\left(\coth \frac{\beta z}{2}\right)$ has poles with residue $\frac{2}{\beta}$ precisely at $z_n = i\omega_n^F$ $(z_n = i\omega_n^B)$.

Proof: (for fermions) $|f(z)| \le |z|^{-(1+\varepsilon)}$ for $|z| \to \infty$ with $\varepsilon > 0$, then

$$0 = \oint_{\Gamma_\infty} \tanh\frac{\beta z}{2}\, f(z)\, dz \overset{\text{residue theorem}}{=}$$



$$= \underbrace{2\pi i \sum_n \operatorname{Res}_{z=z_n}\left(\tanh\frac{\beta z}{2} f(z)\right)}_{= \frac{4\pi i}{\beta} \sum_n f(z_n)} + 2\pi i \sum_s \tanh\frac{\beta z_s}{2} \operatorname{Res}_{z=z_s}\left(f(z)\right)$$

$$\left[\operatorname{Res}_{z=z_n}\left(\tanh\frac{\beta z_n}{2}\right) = \frac{2}{\beta}\right]$$

$$\Longleftrightarrow \quad \frac{1}{\beta} \sum_n f(z_n) = -\frac{1}{2} \sum_s \tanh\frac{\beta z_s}{2} \operatorname{Res}_{z=z_s}\left(f(z)\right). \quad \square$$

Analogous for bosons with $z_n = i\omega_n^B$ and $\tanh \to \coth$.