In equilibrium quantum statistical mechanics, define the density operator to be
\[ \hat{\rho}(\beta) = e^{-\beta \hat{H}}, \quad \beta = \frac{1}{k_B T}, \quad \frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] \]

(in the grand canonical ensemble, replace \( \hat{H} \to \hat{H} - \mu \hat{N} \))

The partition function, in terms of the density operator is
\[ Z(\beta) = \text{Tr} [\hat{\rho}(\beta)] = \text{Tr} e^{-\beta \hat{H}} \]

All thermodynamic quantities follow from the partition function. The ensemble average of an operator, \( \hat{A} \) is defined as:
\[ \langle \hat{A} \rangle_\beta = \frac{1}{Z(\beta)} \text{Tr} [\hat{A} e^{-\beta \hat{H}}] = \frac{1}{Z(\beta)} \text{Tr} [\hat{A} \hat{\rho}] \]

Similarly, the thermal quantum correlation function of two operators \( \hat{A} \) and \( \hat{B} \) is:
\[ \langle \hat{A} \hat{B} \rangle_\beta = \frac{1}{Z(\beta)} \text{Tr} [\hat{A} \hat{B} \hat{\rho}(\beta)] \]

Kubo-Martin-Schwinger relations

For any Schrödinger operator, \( \hat{A} \), one can define a time dependent Heisenberg operator, \( \hat{A}(t) \) defined as:
\[ \hat{A}(t) = e^{i\hat{H}t} \hat{A} e^{-i\hat{H}t} \]

The correlation of two Heisenberg operators is called the thermal quantum time correlation function, and is defined as:
\[ \langle \hat{A}(t) \hat{B}(t) \rangle_\beta = \frac{1}{Z(\beta)} \text{Tr} [\hat{A}(t) \hat{B}(t) \hat{\rho}(\beta)] \]
\[ \langle \hat{A}(t) \hat{B}(t) \rangle_\beta = \frac{1}{Z(\beta)} \operatorname{Tr} \left[ \hat{A}(t) \hat{B}(t) \hat{\rho}(\beta) \right] \]

\[ = \frac{1}{Z(\beta)} \operatorname{Tr} \left[ \hat{A}(t) e^{i\hat{H}t} \hat{B} e^{-i\hat{H}t} e^{-\beta \hat{H}} \right] \]

\[ = \frac{1}{Z(\beta)} \operatorname{Tr} \left[ \hat{A}(t) \hat{\rho}(\beta) e^{i\hat{H}t} \hat{B} e^{-i\hat{H}t} e^{-\beta \hat{H}} \right] \]

\[ = \frac{1}{Z(\beta)} \operatorname{Tr} \left[ \hat{A}(t) \hat{\rho}(\beta) \hat{B}(t-i\beta) \right] \]

\[ = \frac{1}{Z(\beta)} \operatorname{Tr} \left[ \hat{B}(t-i\beta) \hat{A}(t) \hat{\rho}(\beta) \right] = \operatorname{Tr} \left[ \hat{B}(t) \hat{A}(t+i\beta) \hat{\rho}(\beta) \right] \]

(form some steps)

If the two operators are the same, \( \hat{A} = \hat{B} \), but evaluated at different times, we have:

\[ \langle \hat{A}(t) \hat{A}(t') \rangle_\beta = \langle \hat{A}(t-i\beta) \hat{A}(t) \rangle_\beta = \langle \hat{A}(t') \hat{A}(t+i\beta) \rangle_\beta. \]

The goal of equilibrium thermal quantum statistics is to be able to evaluate thermal averages and quantum TCFs. In the presence of interactions, the Hilbert space is very complicated — summing over all states is difficult. Can get around this difficulty by following the Matsubara Formalism (also called imaginary time formalism).

The idea is to introduce a "modified" interaction picture by splitting up the total Hamiltonian into a free part and an interaction part:

\[ \hat{H} = \hat{H}_0 + \hat{H}' \]

(In the grand canonical ensemble, treat the \(-\mu N\) term as part of the free Hamiltonian.)
Then split up the density matrix:

\[ \rho(\beta) = e^{-\beta \hat{H}} = e^{-\beta \hat{H}_0} e^{-\beta \hat{H}'} = \rho_0(\beta) \hat{S}(\beta) \]

(Free part) (Interaction part)

Note that if \( \hat{H}_0 \) commutes with \( \hat{H}' \), then \( \hat{S}(\beta) = e^{\beta \hat{H}_0} e^{-\beta \hat{H}_0} e^{-\beta \hat{H}'} = e^{-\beta \hat{H}'} \)

\[ \hat{S}(\beta) = \rho^{-1}_0(\beta) \hat{p}(\beta) \]

We can then see how the density matrices depend on \( \beta \):

\[ \frac{\partial \rho_0}{\partial \beta} = \frac{\partial}{\partial \beta} e^{-\beta \hat{H}_0} = -\hat{H}_0 e^{-\beta \hat{H}_0} = -\hat{H}_0 \rho_0(\beta) \]

\[ \frac{\partial \hat{p}}{\partial \beta} = \frac{\partial}{\partial \beta} e^{-\beta \hat{H}} = -\hat{H} \rho(\beta) = -(\hat{H}_0 + \hat{H}') \rho(\beta) \]

\[ \frac{\partial \hat{S}}{\partial \beta} = \frac{\partial}{\partial \beta} (e^{\beta \hat{H}_0} e^{-\beta \hat{H}}) = \hat{H}_0 e^{\beta \hat{H}_0} e^{-\beta \hat{H}} - e^{\beta \hat{H}_0} \hat{H} e^{-\beta \hat{H}} \]

\[ = e^{\beta \hat{H}_0} (\hat{H}_0 - \hat{H}) e^{-\beta \hat{H}} \]

\[ = e^{\beta \hat{H}_0} (-\hat{H}') e^{-\beta \hat{H}_0} e^{\beta \hat{H}_0} e^{-\beta \hat{H}} = -\hat{H}_I'(\beta) \hat{S}(\beta) \]

If we interpret \( \rho(\beta) = e^{-\beta \hat{H}} \) as the time evolution operator in the negative imaginary direction, \( t = -i \beta \), \( \hat{S} \) is the time evolution operator in the interaction picture, it note similarity with its equation of motion,

\[ i \hbar \frac{d \hat{U}_I}{dt} = \hat{H}_I(\beta) \hat{U}_I \]

Having introduced \( \hat{H}_I'(\beta) = e^{\beta \hat{H}_0} \hat{H}' e^{-\beta \hat{H}_0} \), we can define the operators in the modified interaction picture as:

\[ \hat{A}_I(\beta) = e^{\beta \hat{H}_0} \hat{A} e^{-\beta \hat{H}_0} = \rho^{-1}_0(\beta) \hat{A} \rho_0(\beta) \]

Cautionary note: The transformation for real \( \beta \) or (negative) imaginary \( t \) is not unitary — must be careful with dealing with such operators.