CORRELATORS, MATSUBARA FREQUENCIES, ETC.

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1. "Imaginary time" evolution

In thermal-equilibrium theory it is very convenient to define a fictitious evolution in a real parameter τ. If $K = H - \mu N$, the Heisenberg evolution of an operator is defined as

$$O_K(\tau) = e^{\frac{1}{\hbar}\tau K} O e^{-\frac{1}{\hbar}\tau K} \tag{1}$$

The evolution is not unitary: $O_K(\tau)^\dagger = O_K^\dagger(-\tau)$.

Exercise 1. Show that, for the simple Hamiltonian $K_0 = \sum_r (\epsilon_r - \mu) c_r^\dagger c_r$, it is

$$\boxed{c_r^\dagger(\tau) = e^{\frac{1}{\hbar}(\epsilon_r-\mu)\tau} c_r^\dagger \qquad c_r(\tau) = e^{-\frac{1}{\hbar}(\epsilon_r-\mu)\tau} c_r}$$

In particular, with $\tau = \hbar\beta$ it is $c_s e^{-\beta K} = e^{-\beta(\epsilon_s-\mu)} e^{-\beta K} c_s$.
It is simple to obtain the thermal averages for bosons $(-)$ and fermions $(+)$:

$$\langle c_r^\dagger c_s \rangle_0 = \frac{\delta_{rs}}{e^{\beta(\epsilon_s-\mu)} \mp 1} \tag{2}$$

$\mathrm{tr}[\rho c_r^\dagger c_s] = \mathrm{tr}[c_s \rho c_r^\dagger] = e^{-\beta(\epsilon_s-\mu)} \mathrm{tr}[\rho c_s c_r^\dagger]$, commute or anticommute. The result follows (this anticipates the derivation of Wick's theorem in thermal theory). □

Exercise 2. Let $A_1 ... A_k$ denote a product of destruction or creation operators of any one-particle states. With $N = \sum_r c_r^\dagger c_r$ show that $e^{\lambda N} A_j e^{-\lambda N} = e^{\pm\lambda} A_j$ with sign $+$ if A_j creates a particle and sign $-$ if it destroys a particle. Then show that if $[K, N] = 0$ it is:

$$\langle A_1 ... A_k \rangle_K = 0$$

if the number of creators is not equal to the number of destructors. In particular k must be even.

1.1. Interaction picture.

Suppose that $K = K_0 + V$. We define the interaction evolution

$$e^{-\frac{1}{\hbar}\tau K} = e^{-\frac{1}{\hbar}\tau K_0} \mathscr{U}(\tau, 0)$$

The operators $\mathscr{U}(\tau, \tau') = \mathscr{U}(\tau, 0)\mathscr{U}(\tau', 0)^{-1}$ have the property of propagators, and solve the Schrödinger-like equation $-\hbar \frac{d}{d\tau} \mathscr{U}(\tau, \tau') = V_{K_0}(\tau) \mathscr{U}(\tau, \tau')$, with formal solution

$$\mathscr{U}(\tau, \tau') = \mathsf{T} \exp -\frac{1}{\hbar} \int_{\tau'}^{\tau} d\tau'' V_{K_0}(\tau'') \tag{3}$$

The T-ordering is defined as the chronological ordering in real time.

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We now obtain a perturbative formula for the gran-canonical potential. With $\tau = \hbar\beta$, we get the useful formula

$$e^{-\beta K} = e^{-\beta K_0}\mathscr{U}(\hbar\beta, 0) \tag{4}$$

The trace gives the partition functions:

$$Z = Z_0\langle \mathscr{U}(\hbar\beta, 0)\rangle_0 \tag{5}$$

the log and the Dyson expansion give a perturbative expansion of the gran-canonical potential:

$$\begin{aligned} \Omega - \Omega_0 =& - k_B T \log\langle \mathscr{U}(\hbar\beta, 0)\rangle_0 \\ =& \langle V\rangle_0 - \frac{k_B T}{2\hbar^2}\iint_0^{\hbar\beta} d\tau_1 d\tau_2 \langle \mathsf{T}\delta V_{K_0}(\tau_1)\delta V_{K_0}(\tau_2)\rangle_0 + ... \end{aligned} \tag{6}$$

where $\langle \ldots\rangle_0$ is the thermal average with K_0.

Exercise 3. If A, B commute under T ordering, show that

$$\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \langle \mathsf{T}A(\tau)B(\tau')\rangle_0 = \hbar\beta \int_0^{\hbar\beta} d\tau \langle A(\tau)B\rangle_0$$

The formula simplifies the second order term of the perturbative expansion of the thermodinamic potential (6). A similar reduction is valid to all orders, and was obtained by Bloch and De Dominicis (1958).

1.2. **The reduction formula.** In thermal theory there is no analogous of a Gell-Mann and Low theorem to obtain the reduction formula. The state of a system is known: it is the Gibbs state.

Let $\psi_1(\tau_1)...\psi_N(\tau_N)$ be a set of field operators evolved with K at different values of τ in the interval $(0, \hbar\beta)$. If $K = K_0 + V$:

$$\boxed{\langle \mathsf{T}\psi_1(\tau_1)...\psi_N(\tau_N)\rangle_K = \frac{\langle \mathsf{T}\mathscr{U}(\hbar\beta, 0)\psi_1(\tau_1)...\psi_N(\tau_N)\rangle_{K_0}}{\langle \mathscr{U}(\hbar\beta, 0)\rangle_{K_0}}} \tag{7}$$

where in the right hand side the operators evolve with K_0.

Proof. First, tau-order the operators, up to a factor $(-1)^p$. Write

$$\psi_K(\tau) = \mathscr{U}(\tau, 0)^{-1}\psi_{K_0}(\tau)\mathscr{U}(\tau, 0)$$

and use $\mathscr{U}(\tau, 0)\mathscr{U}(\tau', 0)^{-1} = \mathscr{U}(\tau, \tau')$. Express the Gibbs state in interaction picture with eqs. (4) and (5). Insert again a T ordering and collect all propagators into a factor $\mathscr{U}(\hbar\beta, 0)$. It is the analogous of the S matrix in zero-temperature. Restore the original order of field operators under the T-ordering. This cancels the permutation sign. □

2. Correlators

We study thermal averages $\langle A(\tau)B(\tau')\rangle = \frac{1}{Z}\text{tr}[e^{-\beta K}A(\tau)B(\tau')]$, with $\tau-$evolution driven by the gran-canonical Hamiltonian K.

Two simple important properties descend from the cyclic property of the trace and the fact that $\tau-$ evolution commutes with the Gibbs operator:

- the correlator is a function of $\tau - \tau'$:

$$\langle A(\tau)B(\tau')\rangle = \langle A(\tau - \tau')B\rangle \tag{8}$$

• the Kubo-Martin-Schwinger (KMS) property:

$$\langle A(\tau)B(\tau')\rangle = \langle B(\tau' + \hbar\beta)A(\tau)\rangle \tag{9}$$

Remark 4. *The KMS property characterizes thermal Gibbs states.*
Proof: *Suppose that a state* ρ *satisfies KMS:* $\mathrm{tr}[\rho A(\tau)B(\tau')] = \mathrm{tr}[\rho B(\tau' + \hbar\beta)A(\tau)]$ *for any pair of operators and parameters. In particular, if* $\tau = \tau' = 0$ *it is* $\mathrm{tr}[\rho AB] = \mathrm{tr}[\rho B(\hbar\beta)A]$. *Then:* $\mathrm{tr}[(B\rho - \rho B(\hbar\beta))A] = 0$. *This (as a Hilbert-Schmidt inner product) implies* $B\rho - \rho B(\hbar\beta) = 0$ *i.e.* $[B, \rho e^{\beta K}] = 0$ *for all* B. *Then* $\rho e^{\beta K}$ *is a multiple of unity, i.e. it is the Gibbs thermal state.* □
(see G. Parisi, Statistical Field Theory).

2.1. **Matsubara frequencies.** Now consider a $\tau-$ordered correlator

$$\begin{aligned} -C^{\mathsf{T}}_{AB}(\tau - \tau') =& \langle \mathsf{T} A(\tau)B(\tau')\rangle \\ =& \theta(\tau - \tau')\langle A(\tau)B(\tau')\rangle \pm \theta(\tau' - \tau)\langle B(\tau')A(\tau)\rangle \end{aligned}$$

where the plus occurs if the correlator is among "Bose-type" operators (ex: a density-density correlator), and the minus occurs if the correlator is among "Fermi-type" ones (ex: a Fermi Green function).
If we restrict times in $0 \le \tau, \tau' \le \hbar\beta$, the correlator C^{T}_{AB} is a function of $\tau - \tau'$ in the interval $[-\hbar\beta, \hbar\beta]$. The Fourier basis on such interval are the orthonormal functions

$$\frac{1}{\sqrt{2\hbar\beta}} e^{-i\omega_n(\tau-\tau')}, \qquad \omega_n = \frac{n\pi}{\hbar\beta}, \qquad n \in \mathbb{Z} \tag{10}$$

where ω_n are named Matsubara frequencies, with the parity of n.

Proposition 5.

$$\boxed{\begin{aligned} C^{\mathsf{T}}_{AB}(\tau - \tau') &= \tfrac{1}{\hbar\beta}\textstyle\sum_n C_{AB}(i\omega_n) e^{-i\omega_n(\tau-\tau')} \\ C_{AB}(i\omega_n) &= \textstyle\int_0^{\hbar\beta} d\sigma\, e^{+i\omega_n\sigma} C^{\mathsf{T}}_{AB}(\sigma) \end{aligned}}$$

where the sum involves even Matsubara frequencies if A *and* B *commute under* T *ordering, odd Matsubara frequencies if the operators anticommute under* T *ordering.*

Proof. The coefficient of the Fourier series is $C_{AB}(i\omega_n) = \frac{1}{2}\int_{-\hbar\beta}^{\hbar\beta} d\sigma e^{+i\omega_n\sigma} C^{\mathsf{T}}_{AB}(\sigma)$. The integral on the negative interval is shifted:

$$C_{AB}(i\omega_n) = \tfrac{1}{2}\int_0^{\hbar\beta} d\sigma e^{i\omega_n\sigma}[C^{\mathsf{T}}_{AB}(\sigma) + (-1)^n C^{\mathsf{T}}_{AB}(\sigma - \hbar\beta)]$$

For $0 \le \sigma \le \hbar\beta$ and the KMS rule: $-C^{\mathsf{T}}_{AB}(\sigma - \hbar\beta) = \langle \mathsf{T} A(\sigma - \hbar\beta)B\rangle = \pm\langle BA(\sigma - \hbar\beta)\rangle = \pm\langle A(\sigma)B\rangle = \mp C^{\mathsf{T}}_{AB}(\sigma)$. Therefore:

$$C_{AB}(i\omega_n) = \tfrac{1}{2}[1 \pm (-1)^n]\int_0^{\hbar\beta} d\sigma e^{i\omega_n\sigma} C^{\mathsf{T}}_{AB}(\sigma)$$

In n is even, the coefficient is identically zero if A, B anticommute, while if n is odd the coefficient is zero if A, B commute. Then only even or odd Matsubara frequencies appear in the sum, according to the statistics of the operators. □

2.2. **Green function of non-interacting particles.**
For $K_0 = \sum_r (\epsilon_r - \mu) c_r^\dagger c_r$ one obtains the Green function for bosons or fermions; n_r is the BE or FD occupation number.

$$-\mathscr{G}^0_{\mu\mu'}(\mathbf{x}\tau, \mathbf{x}'\tau') = \sum_r \langle \mathbf{x}\mu | r\rangle\langle r|\mathbf{x}'\mu'\rangle e^{-\frac{i}{\hbar}(\epsilon_r-\mu)(\tau-\tau')}[\theta(\tau-\tau')(1\pm n_r) \pm \theta(\tau'-\tau)n_r]$$

The frequency expansion is evaluated:

$$\mathscr{G}^0_{\mu\mu'}(\mathbf{x}\tau, \mathbf{x}'\tau') = \frac{1}{\hbar\beta}\sum_n \mathscr{G}^0_{\mu\mu'}(\mathbf{x}, \mathbf{x}', i\omega_n) e^{-i\omega_n(\tau-\tau')} \tag{11}$$

$$\mathscr{G}^0_{\mu\mu'}(\mathbf{x}, \mathbf{x}', i\omega_n) = -\sum_r \langle \mathbf{x}\mu | r\rangle\langle r|\mathbf{x}'\mu'\rangle (1\pm n_r)\int_0^{\hbar\beta} d\sigma e^{-\frac{i}{\hbar}(\epsilon_r-\mu)\sigma}$$

$$= \sum_r \frac{\langle \mathbf{x}\mu | r\rangle\langle r|\mathbf{x}'\mu'\rangle}{i\omega_n - \frac{1}{\hbar}(\epsilon_r - \mu)} \tag{12}$$

In particular, for the ideal gas of non-interacting free bosons or fermions it is:

$$\boxed{\mathscr{G}^0_{\mu\mu'}(k, i\omega_n) = \delta_{\mu\mu'}\frac{1}{i\omega_n - \frac{1}{\hbar}(\epsilon_k - \mu)}}$$

The only difference between bosons and fermions is the parity of the frequency ω_n.

2.3. **Matsubara sums.** Thermal theory involves sums on Matsubara even or odd frequencies, instead of frequency integrals on the real line. An important sum is the following one:

Proposition 6.

$$\boxed{\frac{1}{\hbar\beta}\sum_{\omega_n}\frac{e^{i\omega_n\eta}}{i\omega_n - \frac{1}{\hbar}(\epsilon-\mu)} = \mp\frac{1}{e^{\beta(\epsilon-\mu)}\mp 1}} \tag{13}$$

Proof. This is a simple proof that avoids methods of complex analysis. For non interacting particles, the density in $\mathbf{x}, \mu$ is: $\langle n_\mu(\mathbf{x})\rangle = \sum_r |\langle \mathbf{x}\mu|r\rangle|^2 n(\epsilon_r)$. The same average can be evaluated with the thermal Green function (12):

$$\langle n_\mu(\mathbf{x})\rangle = \mp\mathscr{G}^0_{\mu\mu}(\mathbf{x}\tau, \mathbf{x}\tau^+) = \mp\frac{1}{\hbar\beta}\sum_n e^{i\omega_n\eta}\mathscr{G}^0_{\mu\mu}(\mathbf{x}, \mathbf{x}, i\omega_n)$$

The comparison and the arbitrariness of the functions $\langle \mathbf{x}\mu|r\rangle$ prove the result. Without the convergence factor the series would logarithmically diverge. □

2.4. **An analytic technique.** The two functions (related to Bose and Fermi distributions)

$$n_\mp(z) = \frac{1}{e^{\beta\hbar z}\mp 1}$$

have simple poles at $z_n = i\omega_n$ with n even for n_-, and n odd for n_+. The residues are respectively $\pm 1/(\hbar\beta)$.
For a meromorphic function f that decays at infinity whose poles $\{z_p\}$ differ from the poles of n_- or n_+, consider the integral on a big circle:

$$\oint_C \frac{dz}{2\pi i} e^{\eta z} n_\mp(z) f(z) = \pm\frac{1}{\hbar\beta}\sum_n f(i\omega_n)e^{i\omega_n\eta} + \sum_p \mathrm{Res}(f n_\mp, z_p)$$

The factor $\exp(\eta z)$ with vanishing η ensures convergence on the half-circle in Re$z <$ 0, while $n_\mp$ decays for Re$z > 0$. Since the integral vanishes for infinite radius, we obtain the Matsubara sum:

$$\frac{1}{\hbar\beta}\sum_n f(i\omega_n)e^{i\omega_n\eta} = \mp\sum_p \mathrm{Res}(fn_\mp, z_p)$$

Eq.(13) results with $f(z) = 1/(z - \frac{1}{\hbar}(\epsilon - \mu))$.

Exercise 7. Evaluate the useful thermal series:

$$\frac{1}{\hbar\beta}\sum_n \frac{1}{i\omega_n - \frac{1}{\hbar}(\epsilon-\mu)}\,\frac{1}{i(\omega_n-\nu) - \frac{1}{\hbar}(\epsilon'-\mu)} \tag{14}$$

$$\frac{1}{\hbar\beta}\sum_n \frac{1}{(i\omega_n - \frac{1}{\hbar}(\epsilon-\mu))^2} \tag{15}$$

$$\frac{1}{\hbar\beta}\sum_n e^{i\omega_n\eta}\log\left(i\omega_n - \frac{\epsilon-\mu}{\hbar}\right) \tag{16}$$

The sum with log requires the keyhole path.