Matsubara formalism, Feynman diagrams

Motivation for the Matsubara formalism. At finite temperature $T > 0$, an arbitrary time ordered 2-point correlation function of the operators $A(t)$ and $B(t')$ can be written as

$$C(t, t') = -\langle \mathcal{T}_t\{A(t)B(t')\}\rangle = -\mathrm{Tr}\big[\rho\ \mathcal{T}_t\{A(t)B(t')\}\big] \tag{1}$$

with $\rho = \mathrm{e}^{-\beta K}/Z$, $Z = \mathrm{Tr}[\mathrm{e}^{-\beta K}]$ (the trace running over the Fock space), $\beta = 1/k_B T$, and $K = (H - \mu N)$.

The Boltzmann factor $\mathrm{e}^{-\beta K}$ looks very much like $U(t) = \mathrm{e}^{-iHt}$ (we set $\hbar = 1$ everywhere here), and both satisfy similar differential equations:

$$i\partial_t U = HU \qquad \text{and} \qquad \partial_\beta \rho = -K\rho. \tag{2}$$

We see that β plays a similar role as an imaginary time $t \to -i\beta$. In order to treat thus U and ρ on the same footing, we make first the replacement $t \to -i\tau$ ($\tau \in \mathbb{R}$), and second shift to the operator $K = H - \mu N$ in the evolution of operators (to account for the grand canonical description). We thus introduce a new representation

$$A(\tau) = \mathrm{e}^{\tau K} A \mathrm{e}^{-\tau K}, \tag{3}$$

and we define correlation functions now as

$$C(\tau, \tau') = -\langle \mathcal{T}_\tau\{A(\tau)B(\tau')\}\rangle = -\frac{1}{Z}\mathrm{Tr}\big[\mathrm{e}^{-\beta K}\mathcal{T}_\tau\{A(\tau)B(\tau')\}\big], \tag{4}$$

where $\mathcal{T}_\tau$ is the time order for τ in the same way as $\mathcal{T}_t$ for t. The connection of such functions to real time correlation functions as $C(t, t')$ is the topic of an exercise next week. Note, however, that such $C(\tau, \tau')$ can be used to describe most thermodynamic (static) quantities by choosing appropriate A and B and by letting $\tau' \to \tau \pm 0$.

With $H = H_0 + V$ (i.e. $K = K_0 + V$), we can define an interaction representation

$$\hat{A}(\tau) = \mathrm{e}^{\tau K_0} A \mathrm{e}^{-\tau K_0} \tag{5}$$

and the evolution operator becomes $\hat{U}(\tau, \tau') = \mathrm{e}^{\tau K_0}\mathrm{e}^{-(\tau-\tau')K}\mathrm{e}^{-\tau' K_0}$, from which follows

$$\partial_\tau \hat{U}(\tau, \tau') = -\hat{V}(\tau)\hat{U}(\tau, \tau'). \tag{6}$$

Exercise 1 (3 points)

(a) Show that

$$\hat{U}(\tau, \tau') = \mathcal{T}_\tau\left[\exp\left(-\int_{\tau'}^{\tau} \mathrm{d}\tau''\ \hat{V}(\tau'')\right)\right] \tag{7}$$

and that

$$C(\tau, \tau') = -\langle \mathcal{T}_\tau\{A(\tau)B(\tau')\}\rangle = -\frac{\langle \mathcal{T}_\tau\{\hat{U}(\beta, 0)\hat{A}(\tau)\hat{B}(\tau')\}\rangle_0}{\langle \hat{U}(\beta, 0)\rangle_0}, \tag{8}$$

where $\langle ...\rangle_0 = \mathrm{Tr}\{\mathrm{e}^{-\beta K_0}(...)\}/Z_0$ and $Z_0 = \mathrm{Tr}\{\mathrm{e}^{-\beta K_0}\}$. This looks very much like the expression obtained by the Gell-Mann–Low formula (yet without subtleties because the denominator appears just from the normalization by Z). This expression allows us to derive a perturbative expansion for thermodynamic averages in the same way as for the time dependent quantum mechanical correlation functions. ***If*** K_0 is quadratic in the creation/annihilation operators ($\sim$ free particles) then the Wick theorem as proved last week applies. The denominator takes into account the cancellation of disconnected diagrams.

(b) Show that $C(\tau, \tau') = C(\tau - \tau')$. (Use (3) and the cyclic property of the trace.)

(c) Show that convergence of $C(\tau)$ [setting $\tau' = 0$] can only be assured for $-\beta < \tau < \beta$: Choose a basis $\{|n\rangle\}$ such that $K|n\rangle = E_n|n\rangle$ and write the trace as $\mathrm{Tr}[...] = \sum_n \langle n|...|n\rangle$, and then insert a completeness relation $\mathbb{1} = \sum_m |m\rangle\langle m|$ between the operators A and B. Observe that the values E_n are bounded below but generally can become arbitrarily large for positive values. Treat $\tau > 0$ and $\tau < 0$ separately.

(d) Show, again using the cyclic property of the trace, that for $-\beta < \tau < 0$

$$C(\tau + \beta) = \pm C(\tau) \qquad [+ : \text{bosons}, - : \text{fermions}] \tag{9}$$

Exercise 2 (1 point) Fourier transform.
Since $-\beta < \tau < \beta$ and we have the periodicity (9), $C(\tau)$ can be expressed by a discrete Fourier sum

$$C(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-i\pi n\tau/\beta} C(n) \qquad C(n) = \frac{1}{2} \int_{-\beta}^{\beta} \mathrm{d}\tau \; \mathrm{e}^{i\pi n\tau/\beta} C(\tau). \tag{10}$$

Using (9), show that for bosons only even n and for fermions only odd n give nonzero $C(n)$. This allows us to define the **Matsubara frequencies**

$$\omega_n = \frac{2n\pi}{\beta} \text{ (bosons)}, \qquad \omega_n = \frac{(2n+1)\pi}{\beta} \text{ (fermions)}, \tag{11}$$

such that (the notation with the $i\omega_n$ is a convention used throughout in the literature)

$$C(i\omega_n) = \int_0^\beta \mathrm{d}\tau \; \mathrm{e}^{i\omega_n \tau} C(\tau), \qquad C(\tau) = \frac{1}{\beta} \sum_{\omega_n} \mathrm{e}^{-i\omega_n \tau} C(i\omega_n). \tag{12}$$

Exercise 3 (3 points) Connection to retarded functions: Wick rotation.

(a) Let us define the retarded function

$$C^r(t) = -i\theta(t)\langle \big[A(t)\,,\, B(0)\big]_{\pm}\rangle \qquad [- : \text{bosons}, + : \text{fermions}], \tag{13}$$

with $A(t) = \mathrm{e}^{iKt} A \mathrm{e}^{-iKt}$. Show that the Fourier transforms $C(i\omega_n)$ and $C^r(\omega)$ (for $t \to \omega$ the regular time-frequency Fourier transformation) describe the same analytic function $\mathcal{C}(z)$ such that $C(i\omega_n) = \mathcal{C}(z = i\omega_n)$ and $C^r(\omega) = \mathcal{C}(z = \omega + i\eta)$.

This means if, for instance, $C(i\omega_n)$ is known, $C^r(\omega)$ can be obtained by the analytic continuation $i\omega_n \to \omega + i\eta$. This is known as the **Wick rotation** (not to be confused with the Wick theorem!).

Hint: Use the basis vectors $|n\rangle$ to write down $C(\tau)$ and $C^r(t)$ in a similar way as in Exercise 1 (c). Then explicitly perform the Fourier transform. Stop here and compare.

(b) What changes if now $A(t) = \mathrm{e}^{iHt} A \mathrm{e}^{-iHt}$ (i.e. using H and no longer K)? Consider concretely the example $A = c_k$ and $B = c_k^\dagger$.

Exercise 4 (3 points) Feynman diagrams.

Let $\hat{V}(t)$ be the electron-electron interaction in the perturbative expansion for the electron Green's function $G^c_\sigma(\mathbf{k}, t - t')$. Evaluate the term in the expansion at order $\hat{V}$, by drawing and labeling the Feynman diagrams and writing down the corresponding equations in $(\mathbf{k}, t)$ and $(\mathbf{k}, \omega)$ space (but do not explicitly calculate the integrals). Also draw and label all connected diagrams at order $\hat{V}^2$ in $(\mathbf{k}, t)$ and $(\mathbf{k}, \omega)$ space.