

10 Lesson 10

10.1 Quantum Statistical Mechanics

10.1.1 Back to KMS – QM at finite T

Let's recall the Boltzmann-Gibbs weight,

$$\hat{\rho} \propto e^{-\beta \hat{H}}. \quad (10.1)$$

This has the same functional expression as the evolution operator,

$$U(t) = e^{-\frac{i}{\hbar} \hat{H} t}. \quad (10.2)$$

Therefore, the weight can be formally written as

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}} = \frac{1}{Z} U(-i\hbar\beta). \quad (10.3)$$

In other words, it is statistical mechanics as a kind of imaginary time QM.

We would identify

$$Z = \text{Tr } U(-i\hbar\beta), \quad (10.4)$$

and an expectation value of an operator

$$\langle \hat{A} \rangle = \frac{\text{Tr} (U(-i\hbar\beta) \hat{A})}{\text{Tr } U(-i\hbar\beta)}. \quad (10.5)$$

Aficionados of Spacial Relativity and QED: this is called the “proper time method”. It was developed by Schwinger, Feinman, Fock, and $\frac{1}{2}$ Fock.

10.1.2 Generalizations

Let's look on an analytic continuation of time to the complex plane. Define a “time” τ through $\frac{it}{\hbar} \leftrightarrow \tau$. This τ has dimensions of [1/Energy]. Generalize $T = 0$ of QM:

$$\left\{ \begin{array}{l} \text{Schroedinger eq.} \\ \text{Heisenberg eq.} \\ \text{S-matrix} \\ \text{Permutation theory} \end{array} \right.$$

Example.

- The Shroedinger representation:

$$H |\psi_s\rangle = i\hbar \frac{\partial}{\partial t} |\psi_s\rangle \longleftrightarrow H |\psi_s\rangle = \frac{\partial}{\partial \tau} |\psi_s\rangle \quad (10.6a)$$

$$|\psi_s(\tau)\rangle = e^{-H\tau} |\psi_s(0)\rangle \quad (10.6b)$$

- The Heisenberg representation:

$$|\psi_H(\tau)\rangle = |\psi_s(0)\rangle \quad (10.7a)$$

$$A_H(\tau) = e^{H\tau} A_S e^{-H\tau} \quad (10.7b)$$

$$\frac{\partial A_H}{\partial \tau} = [H, A_H] \quad (10.7c)$$

Remark. The de Boglie wavelength:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = \frac{\partial}{\partial \tau} \psi. \quad (10.8)$$

- Ext. in space: $\nabla^2 \psi \sim \frac{\psi}{\lambda^2}$;
- Ext. in time: $\frac{\partial \psi}{\partial \tau} \sim \frac{\psi}{\beta}$
- Hence, $\lambda^2 \sim \beta$, or $\lambda^{-1} = \sqrt{\frac{2mk_B T}{\hbar^2}}$.

10.1.3 Free Particle Hamiltonian

Let's inspect

$$H = \sum_k \varepsilon_k c_k^\dagger c_k, \quad (10.9)$$

such that

$$\begin{cases} \frac{\partial c_k}{\partial \tau} = [H, c_k] = -\varepsilon_k c_k, \\ \frac{\partial c_k^\dagger}{\partial \tau} = [H, c_k^\dagger] = +\varepsilon_k c_k^\dagger. \end{cases} \quad (10.10)$$

Therefore

$$\begin{cases} c_k(\tau) = e^{-\varepsilon_k \tau} c_k(0) \\ c_k^\dagger(\tau) = e^{-\varepsilon_k \tau} c_k^\dagger(0). \end{cases} \quad (10.11)$$

The operators c_k^\dagger and c_k are no longer Hermitian conjugates.

10.1.4 Interaction Representation

Here, $H = H_0 + V$, and we freeze the time evolution associated to H_0 :

$$\begin{aligned} |\psi_I(\tau)\rangle &= e^{H_0 \tau} |\psi_S(\tau)\rangle \\ &= e^{H_0 \tau} e^{-H \tau} |\psi_H\rangle \\ &\equiv U(\tau) |\psi_H\rangle. \end{aligned} \quad (10.12)$$

Here

$$\begin{aligned} |\psi_I(\tau_1)\rangle &= U(\tau_1) U^{-1}(\tau_2) |\psi_I(\tau_2)\rangle \\ &\equiv \underbrace{S(\tau_1, \tau_2)}_{S\text{-matrix}} |\psi_I(\tau_2)\rangle, \end{aligned} \quad (10.13)$$

and we have defined the S -matrix. Now,

$$\begin{aligned} -\frac{\partial}{\partial \tau} U(\tau) &= -\frac{\partial}{\partial \tau} (e^{H_0 \tau} e^{-H \tau}) = e^{H_0 \tau} V e^{-H \tau} \\ &= e^{H_0 \tau} V e^{-H_0 \tau} U(\tau) \equiv V_I(\tau) U(\tau). \end{aligned} \quad (10.14)$$

Hence,

$$-\frac{\partial}{\partial \tau_1} S(\tau_1, \tau_2) = V_I(\tau_1) S(\tau_1, \tau_2). \quad (10.15)$$

We would therefore write U and S in a time-ordered manner:

$$U(\tau) = \mathcal{T} \exp \left[-\int_0^\tau d\tau' V_I(\tau') \right], \quad (10.16)$$

$$S(\tau_1, \tau_2) = \mathcal{T} \exp \left[-\int_{\tau_1}^{\tau_2} d\tau' V_I(\tau') \right]. \quad (10.17)$$

10.1.5 A Straightforward Consequence: Peierls Perturbation Th.

Let's inspect the partition function

$$\begin{aligned} Z &= \text{Tr} (e^{-\beta H}) = \text{Tr} (e^{-\beta H_0} U(\beta)) \\ &= \underbrace{\text{Tr} (e^{-\beta H_0})}_{Z_0} \frac{\text{Tr} (e^{-\beta H_0} U(\beta))}{\underbrace{\text{Tr} (e^{-\beta H_0})}_{\langle U(\beta) \rangle_0}}. \end{aligned} \quad (10.18)$$

Therefore we define this partition as a time ordering on the interaction

$$\frac{Z}{Z_0} = e^{-\beta \Delta F} = \left\langle \mathcal{T} \exp \left[-\int_0^\beta d\tau' V_I(\tau') \right] \right\rangle_0. \quad (10.19)$$

This is an exact relation. It can be solved using a perturbation approach.

10.1.6 Imaginary Time Green's Function

Let's inspect the quantum fields $\hat{\psi}_\lambda(\tau)$ with quantum number λ . Let us define

$$G_{\lambda\lambda'}(\tau, \tau') \equiv -\left\langle \mathcal{T} \hat{\psi}_\lambda(\tau) \hat{\psi}_{\lambda'}^\dagger(\tau') \right\rangle = \text{Tr} \left(e^{-\beta(H-F)} \hat{\psi}_\lambda(\tau) \hat{\psi}_{\lambda'}^\dagger(\tau') \right), \quad (10.20)$$

where the average $\langle \cdot \rangle$ is wrt. H , \mathcal{T} is the time ordering operator, and $F \equiv -T \ln Z$.

Remark. Provided that H is time independent, we have $G_{\lambda\lambda'}(\tau - \tau')$. In most cases, the quantum number λ is conserved:

$$G_{\lambda\lambda'}(\tau - \tau') = \delta_{\lambda\lambda'} G_\lambda(\tau - \tau'). \quad (10.21)$$

10.1.7 Non-interacting Systems

In non-interacting system with Hamiltonian

$$H = \sum_\lambda \varepsilon_\lambda \hat{\psi}_\lambda^\dagger \hat{\psi}_\lambda, \quad \varepsilon_\lambda = \underbrace{E_\lambda}_{\text{single particle energies}} - \mu. \quad (10.22)$$

Let us seek the expectation value of

$$\left\langle \hat{\psi}_\lambda^\dagger \hat{\psi}_{\lambda'} \right\rangle = \delta_{\lambda\lambda'} \times \begin{cases} n(\varepsilon_\lambda) & \text{bosons} \\ f(\varepsilon_k) & \text{fermions} \end{cases}. \quad (10.23)$$

where we have defined the occupation probabilities by

$$n(\varepsilon_\lambda) = \frac{1}{e^{\beta\varepsilon_\lambda} - 1}, \quad f(\varepsilon_\lambda) = \frac{1}{e^{\beta\varepsilon_\lambda} + 1}. \quad (10.24)$$

In a similar matter,

$$\left\langle \hat{\psi}_\lambda \hat{\psi}_{\lambda'}^\dagger \right\rangle = \delta_{\lambda\lambda'} \pm \left\langle \hat{\psi}_\lambda^\dagger \hat{\psi}_{\lambda'} \right\rangle = \delta_{\lambda\lambda'} \times \begin{cases} 1 + n(\varepsilon_\lambda) & \text{bosons} \\ 1 - f(\varepsilon_k) & \text{fermions} \end{cases}. \quad (10.25)$$

Using the time evolution of the operators

$$\begin{cases} \hat{\psi}_\lambda(\tau) = e^{-\varepsilon_\lambda \tau} \hat{\psi}_\lambda(0) \\ \hat{\psi}_\lambda^\dagger(\tau) = e^{-\varepsilon_\lambda \tau} \hat{\psi}_\lambda^\dagger(0) \end{cases}, \quad (10.26)$$

we will obtain the Green's function

$$G_{\lambda\lambda'}(\tau - \tau') = -\left[\Theta(\tau - \tau') \left\langle \hat{\psi}_\lambda \hat{\psi}_{\lambda'}^\dagger \right\rangle + \varphi \Theta(\tau' - \tau) \left\langle \hat{\psi}_{\lambda'}^\dagger \hat{\psi}_\lambda \right\rangle \right] e^{-\varepsilon_\lambda(\tau - \tau')}, \quad (10.27)$$

where $\Theta(\tau - \tau')$ is the time ordering operator and

$$\varphi = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions.} \end{cases} \quad (10.28)$$

Therefore,

$$G_{\lambda\lambda'}(\tau - \tau') = -\left[\Theta(\tau - \tau') \left\langle \hat{\psi}_\lambda(\tau) \hat{\psi}_{\lambda'}^\dagger(\tau') \right\rangle \pm \Theta(\tau' - \tau) \left\langle \hat{\psi}_{\lambda'}^\dagger(\tau') \hat{\psi}_\lambda(\tau) \right\rangle \right]. \quad (10.29)$$

Consider

$$\begin{aligned} G_{\lambda\lambda'}(\tau) &= -\varphi \left\langle \hat{\psi}_{\lambda'}^\dagger(0) \hat{\psi}_\lambda(\tau) \right\rangle \\ &= -\varphi \text{Tr} \left(e^{-\beta(H-F)} \hat{\psi}_{\lambda'}^\dagger e^{\tau H} \hat{\psi}_\lambda e^{-\tau H} \right) \\ &= -\varphi \text{Tr} \left(e^{\tau H} \hat{\psi}_\lambda e^{-\tau H} e^{-\beta(H-F)} \hat{\psi}_{\lambda'}^\dagger \right) \\ &= -\varphi \text{Tr} \left(e^{\beta F} e^{\tau H} \hat{\psi}_\lambda e^{-(\tau+\beta)H} \hat{\psi}_{\lambda'}^\dagger \right) \\ &= -\varphi \text{Tr} \left(e^{-\beta(H-F)} e^{(\tau+\beta)H} \hat{\psi}_\lambda e^{-(\tau+\beta)H} \hat{\psi}_{\lambda'}^\dagger \right), \end{aligned} \quad (10.30)$$

where from the 3rd to the 4th line we demanded $\tau + \beta > 0$ so that the operator is trace class. Hence

$$G_{\lambda\lambda'}(\tau) = -\varphi \left\langle \hat{\psi}_\lambda(\tau + \beta) \hat{\psi}_{\lambda'}^\dagger(0) \right\rangle = \varphi G_{\lambda\lambda'}(\tau + \beta), \quad (10.31)$$

or

$$\boxed{G_{\lambda\lambda'}(\tau) = \varphi G_{\lambda\lambda'}(\tau + \beta)}, \quad -\beta < \tau < 0. \quad (10.32)$$

Corollary. *The imaginary time Green's function is either periodic (bosons) or anti-periodic (fermions) wrt. τ .*

10.1.8 Fourier Series Expansion – Matsubara Frequencies

Let us define

$$\begin{cases} \nu_n = \frac{2\pi n}{\beta} & \text{bosons} \\ \omega_n = \frac{\pi(2n+1)}{\beta} & \text{fermions,} \end{cases} \quad (10.33)$$

so that

$$\begin{cases} e^{i\nu_n(\tau+\beta)} = e^{i\nu_n\tau} & \text{bosons} \\ e^{i\omega_n(\tau+\beta)} = e^{i\omega_n\tau} e^{i\pi(2n+1)} = -e^{i\omega_n\tau} & \text{fermions.} \end{cases} \quad (10.34)$$

Hence

$$G_{\lambda\lambda'}(\tau) = \begin{cases} \sum_{-\infty}^{\infty} G_{\lambda\lambda'}(\nu_n) e^{-i\nu_n\tau} & \text{bosons} \\ \sum_{-\infty}^{\infty} G_{\lambda\lambda'}(\omega_n) e^{-i\omega_n\tau} & \text{fermions.} \end{cases} \quad (10.35)$$

10.1.9 Simple Examples

Free fermions or bosons:

$$G_{\lambda\lambda'}(\tau) = -e^{-i\varepsilon_\lambda\tau} \times \begin{cases} (1 + n(\varepsilon_\lambda)) \Theta(\tau) + n(\varepsilon_\lambda) \Theta(-\tau) & \text{bosons} \\ (1 - f(\varepsilon_k)) \Theta(\tau) - f(\varepsilon_\lambda) \Theta(-\tau) & \text{fermions.} \end{cases} \quad (10.36)$$

For fermions we have

$$\begin{aligned} G_\lambda(\omega_n) &= - \int_0^\beta d\tau e^{(i\omega_n - \varepsilon_\lambda)\tau} (1 - f(\varepsilon_k)) \\ &= - \frac{1}{i\omega_n - \varepsilon_\lambda} \frac{e^{(i\omega_n - \varepsilon_\lambda)\beta} - 1}{1 + e^{-\beta\varepsilon_\lambda}} = - \frac{1}{i\omega_n - \varepsilon_\lambda} (-1) \frac{e^{-\varepsilon_\lambda\beta} + 1}{1 + e^{-\beta\varepsilon_\lambda}}, \end{aligned} \quad (10.37)$$

Or

$$G_\lambda(\omega_n) = \frac{1}{i\omega_n - \varepsilon_\lambda}, \quad \text{fermions.} \quad (10.38a)$$

Similarly, for bosons,

$$G_\lambda(\nu_n) = \frac{1}{i\nu_n - \varepsilon_\lambda}, \quad \text{bosons.} \quad (10.38b)$$