Appendix A2

A2.1. The Two-Point Function: Spectral Representation

In the low temperature ($\beta \to \infty$) limit, the 2-point correlation function

$$Z^{(2)}(\tau) = \langle q(0)\, q(\tau) \rangle \qquad (\tau = it/\hbar > 0)$$

$$= \frac{1}{\mathcal{Z}(\beta)} \mathrm{tr}\left(e^{-(\beta-\tau)H} \hat{q}\, e^{-\tau H} \hat{q} \right) \qquad \text{[see eq(2.38)]}$$

reduces to

$$Z^{(2)}(\tau) \approx \left\langle 0 \,\middle|\, e^{\tau H} \hat{q}\, e^{-\tau H} \hat{q} \,\middle|\, 0 \right\rangle$$

$$= \left\langle 0 \,\middle|\, \hat{q}\, e^{-\tau(H-\varepsilon_0)} \hat{q} \,\middle|\, 0 \right\rangle \qquad \text{[see eq(2.40)]}$$

$$= \left\langle 0 \,\middle|\, \hat{q}\, e^{-\tau H} \hat{q}\, e^{\tau H} \,\middle|\, 0 \right\rangle$$

where ε_0 is the ground state energy so that $H \mid 0 \rangle = \varepsilon_0 \mid 0 \rangle$.

From eq(2.38), we see that $\langle q(\tau_1)\, q(\tau_2) \rangle$ is a function of $\tau_2 - \tau_1$. We can relax the restriction $\tau_2 > \tau_1$ & write

$$\langle q(\tau)\, q(0) \rangle = \langle q(0)\, q(-\tau) \rangle \qquad (\tau > 0)$$

$$= \frac{1}{\mathcal{Z}(\beta)} \mathrm{tr}\left(e^{-(\beta-\tau)H} \hat{q}\, e^{-\tau H} \hat{q} \right)$$

$$\underset{\beta\to\infty}{=} \left\langle 0 \,\middle|\, \hat{q}\, e^{-\tau H} \hat{q}\, e^{\tau H} \,\middle|\, 0 \right\rangle$$

Combining the two cases, we can write, for unrestricted τ,

$$Z^{(2)}(\tau) = \langle q(0)\, q(\tau) \rangle$$

$$\underset{\beta\to\infty}{=} \left\langle 0 \,\middle|\, \hat{q}\, e^{-|\tau| H} \hat{q}\, e^{|\tau| H} \,\middle|\, 0 \right\rangle \qquad \text{(A2.1a)}$$

Assume H to be hermitian with a discrete spectrum that is bounded below so that

$$H \mid n \rangle = \varepsilon_n \mid n \rangle \qquad \text{with} \qquad n \ge 0$$

we have

$$Z^{(2)}(\tau) \underset{\beta\to\infty}{=} \sum_n \left\langle 0 \,\middle|\, \hat{q}\, e^{-|\tau| H} \,\middle|\, n \right\rangle \left\langle n \mid \hat{q} \mid 0 \right\rangle e^{|\tau|\,\varepsilon_0}$$

$$= \sum_n \left\langle 0 \mid \hat{q} \mid n \right\rangle \left\langle n \mid \hat{q} \mid 0 \right\rangle e^{-|\tau|(\varepsilon_n - \varepsilon_0)}$$

$$= \sum_n \left| \left\langle 0 \mid \hat{q} \mid n \right\rangle \right|^2 e^{-|\tau|(\varepsilon_n - \varepsilon_0)} \qquad \text{(A2.1)}$$

For $|\tau| \to \infty$, only the $n = 0$ term survives,

$$Z^{(2)}(\tau) \approx \left| \left\langle 0 \mid \hat{q} \mid 0 \right\rangle \right|^2$$

which can be removed by changing to the new variable

$$\hat{r} = \hat{q} - \left\langle 0 \mid \hat{q} \mid 0 \right\rangle = \hat{q} - q_0 \qquad \text{where} \qquad q_0 = \left\langle 0 \mid \hat{q} \mid 0 \right\rangle$$

Thus, using

$$\langle 0 \mid q_0 \mid 0 \rangle = q_0 \langle 0 \mid 0 \rangle = q_0$$

we have

$$Z^{(2)}(\tau) = \langle r(0)\, r(\tau) \rangle$$

$$= \left| \left\langle 0 \mid \hat{r} \mid 0 \right\rangle \right|^2$$

$$= \left| \left\langle 0 \mid \hat{q} \mid 0 \right\rangle - \langle 0 \mid q_0 \mid 0 \rangle \right|^2$$

$$= \mid q_0 - q_0 \mid^2 = 0$$

The Fourier transform is

$$\tilde{Z}^{(2)}(\omega) = \int d\tau\, Z^{(2)}(\tau)\, e^{i\omega\tau}$$

$$= \sum_n \left| \langle 0 \mid \hat{q} \mid n \rangle \right|^2 \int_{-\infty}^{\infty} dt\; e^{-(\varepsilon_n - \varepsilon_0)\,|\tau|}\; e^{i\omega\tau}$$

Reminder: since $[\tau] = [E]^{-1}$, $[\omega] = [E]$, where $[x]$ = dimension of x & E = energy.

For $x > 0$, we have

$$\int_{-\infty}^{\infty} d\tau\, e^{-x|\tau|}\; e^{i\omega\tau} = \int_{-\infty}^{0} d\tau\; e^{(i\omega + x)\tau} + \int_{0}^{\infty} d\tau\; e^{(i\omega - x)\tau}$$

$$= \frac{1}{i\omega + x} - \frac{1}{i\omega - x}$$

$$= \frac{2x}{\omega^2 + x^2}$$

Furthermore

$$\int_{-\infty}^{\infty} d\tau\; e^{i\omega\tau} = 2\pi\,\delta(\omega)$$

$$\rightarrow \qquad \tilde{Z}^{(2)}(\omega) = 2\pi\,\delta(\omega) \left| \langle 0 \mid \hat{q} \mid 0 \rangle \right|^2 + \sum_{n>0} \frac{2(\varepsilon_n - \varepsilon_0)}{\omega^2 + (\varepsilon_n - \varepsilon_0)^2} \left| \langle 0 \mid \hat{q} \mid n \rangle \right|^2 \qquad \text{(A2.2)}$$

Besides the delta function singularity at $\omega = 0$, all poles of $\tilde{Z}^{(2)}(\omega)$ as a function of ω^2 are on the negative real axis, i.e.,

$$\omega^2 = -(\varepsilon_n - \varepsilon_0)^2 < 0$$

with residues

$$2(\varepsilon_n - \varepsilon_0) \left| \langle 0 \mid \hat{q} \mid n \rangle \right|^2$$

that are real & positive. Thus, $\tilde{Z}^{(2)}(\omega)$ cannot decay faster than $\frac{1}{\omega^2}$ as $\omega^2 \to \infty$.

From (A2.1a), we have, for $\tau > 0$,

$$\frac{d}{d\tau} Z^{(2)}(\tau) = \frac{d}{d\tau} \langle 0 \mid \hat{q}\, e^{-\tau H}\, \hat{q}\, e^{\tau H} \mid 0 \rangle$$

$$= \langle 0 \mid \left(-\hat{q}\, e^{-\tau H} H\, \hat{q}\, e^{\tau H} + \hat{q}\, e^{-\tau H}\, \hat{q}\, H\, e^{\tau H} \right) \mid 0 \rangle$$

$$= \langle 0 \mid \hat{q}\, e^{-\tau H} [\hat{q}, H]\, e^{\tau H} \mid 0 \rangle$$

$$\rightarrow \qquad \lim_{\tau \to 0_+} \frac{d}{d\tau} Z^{(2)}(\tau) = \langle 0 \mid \hat{q}\,[\hat{q}, H] \mid 0 \rangle$$

The complex conjugate of the L.H.S. is

$$\langle 0 \mid \hat{q}\,[\hat{q}, H] \mid 0 \rangle^* = \langle 0 \mid (\hat{q}\,[\hat{q}, H])^+ \mid 0 \rangle$$

$$= \langle 0 \mid [H, \hat{q}]\,\hat{q} \mid 0 \rangle$$

$$= -\langle 0 \mid [\hat{q}, H]\,\hat{q} \mid 0 \rangle$$

Since $Z^{(2)}$ is real , we have

$$\lim_{\tau \to 0_+} \frac{d}{d\tau} Z^{(2)}(\tau) = \frac{1}{2} \left\{ \langle 0 \mid \hat{q}\,[\hat{q}, H] \mid 0 \rangle - \langle 0 \mid [\hat{q}, H]\,\hat{q} \mid 0 \rangle \right\}$$

$$= \frac{1}{2} \langle 0 \mid [\hat{q}, [\hat{q}, H]] \mid 0 \rangle$$

For

$$H = \frac{\hat{p}^2}{2m} + V(q)$$

we have

$$[\hat{q}, H] = \left[\hat{q}, \frac{\hat{p}^2}{2m}\right] = \frac{1}{2m} \{\hat{p}[\hat{q}, \hat{p}] + [\hat{q}, \hat{p}]\hat{p}\} = \frac{i\hbar}{m} \hat{p}$$

$$\rightarrow \qquad [\hat{q}, [\hat{q}, H]] = \frac{i\hbar}{m} [\hat{q}, \hat{p}] = -\frac{\hbar^2}{m}$$

Hence,

$$\lim_{\tau \to 0_+} \frac{d}{d\tau} Z^{(2)}(\tau) = -\frac{\hbar^2}{2m}$$

From eq(A2.1), we have, for $\beta \to \infty$ & $\tau > 0$,

$$\frac{d}{d\tau} Z^{(2)}(\tau) = -\sum_n (\varepsilon_n - \varepsilon_0) \left|\langle 0 \mid \hat{q} \mid n \rangle\right|^2 e^{-\tau(\varepsilon_n - \varepsilon_0)}$$

$$\rightarrow \qquad \lim_{\tau \to 0_+} \frac{d}{d\tau} Z^{(2)}(\tau) = -\sum_n (\varepsilon_n - \varepsilon_0) \left|\langle 0 \mid \hat{q} \mid n \rangle\right|^2$$

$$\therefore \qquad \frac{\hbar^2}{2m} = \sum_n (\varepsilon_n - \varepsilon_0) \left|\langle 0 \mid \hat{q} \mid n \rangle\right|^2$$

Thus, for $\omega \to \infty$, eq(A.2.2) becomes

$$\tilde{Z}^{(2)}(\omega) = \sum_{n>0} \frac{2(\varepsilon_n - \varepsilon_0)}{\omega^2} \left|\langle 0 \mid \hat{q} \mid n \rangle\right|^2$$

$$= \frac{\hbar^2}{m\,\omega^2}$$