# 12.2: Kubo Transform Expression for the Time Correlation Function

We shall derive the following expression for the quantum time correlation function

$$\Phi_{AB}(t) = \int_0^\beta d\lambda\ \langle \dot{B}(-i\hbar\lambda)A(t)\rangle_0$$

known as a **Kubo transform** relation. Since $\dot{B}$ is given by the Heisenberg equation:

$$\dot{B} = \frac{1}{i\hbar}[B, H_0]$$

it follows that

$$\dot{B}(t) = -\frac{1}{i\hbar}e^{iH_0t/\hbar}[H_0, B(0)]e^{-iH_0t/\hbar}$$

Evaluating the expression at $t = -i\hbar\lambda$ gives

$$\dot{B}(-i\hbar\lambda) = e^{\lambda H_0}\frac{1}{i\hbar}[B(0), H_0]e^{-\lambda H_0}$$

Thus,

$$\Phi_{AB}(t) = \int_0^\beta d\lambda \langle e^{\lambda H_0}\left(\frac{1}{i\hbar}[B(0), H_0]\right) e^{-\lambda H_0}A(t)\rangle_0$$

By performing the trace in the basis of eigenvectors of $H_0$, we obtain

$$\begin{aligned}
\Phi_{AB}(t) &= \frac{1}{Q}\int_0^\beta d\lambda \sum_n \langle n|e^{\lambda H_0}\left(\frac{1}{i\hbar}\right)[B(0), H_0]e^{-\lambda H_0}A(t)|n\rangle e^{-\beta E_n} \\
&= \frac{1}{Q}\int_0^\beta d\lambda \sum_{m,n} \langle n|e^{\lambda H_0}\left(\frac{1}{i\hbar}\right)[B(0), H_0]\, e^{-\lambda H_0}|m\rangle\langle m|A(t)|n\rangle e^{-\beta E_n} \\
&= \frac{1}{Q}\int_0^\beta d\lambda \sum_{m,n} e^{\lambda E_n}e^{-\lambda E_m}\frac{1}{i\hbar}\langle n|[B(0), H_0]|m\rangle\langle m|A(t)|n\rangle e^{-\beta E_n} \\
&= \frac{1}{Q}\sum_{m,n} e^{-\beta E_n}\frac{e^{\beta(E_n - E_m)} - 1}{(E_n - E_m)}\frac{1}{i\hbar}\langle n|[B(0), H_0]|m\rangle\langle m|A(t)|n\rangle e^{-\beta E_n}
\end{aligned}$$

But

$$\langle n|[B(0), H_0]|m\rangle = \langle n|B(0)H_0 - H_0B(0)|m\rangle = (E_m - E_n)\langle n|B(0)|m\rangle$$

Therefore,

$$\begin{aligned}
\Phi_{AB}(t) &= -\frac{1}{i\hbar Q}\sum_{m,n}\left(e^{-\beta E_n} - e^{-\beta E_m}\right)\langle n|B(0)|m\rangle\langle m|A(t)|n\rangle \\
&= -\frac{1}{i\hbar Q}\left[\sum_{m,n} e^{-\beta E_m}\langle m|A(t)|n\rangle\langle n|B(0)|m\rangle - \sum_{m,n} e^{-\beta E_n}\langle n|B(0)|m\rangle\langle m|A(t)|n\rangle\right] \\
&= \frac{i}{\hbar}\langle [A(t), B(0)]\rangle_0
\end{aligned}$$

which proves the relation. The classical limit can be deduced easily from the Kubo transform relation:

$$\Phi_{AB}(t) \longrightarrow \beta\langle \dot{B}(0)A(t)\rangle_0$$

Note further, by using the cylic properties of the trace, that

$$\langle\dot{B}(-i\hbar\lambda)B(t)\rangle_0 = -\frac{d}{dt}\langle B(-i\hbar\lambda)B(t)\rangle_0$$