Correlation function (energy gap) and its symmetries

$$g(t) = \int_0^t d\tau \int_0^\tau d\tau' \, C(\tau')$$

$$C(t) = \frac{1}{\hbar^2} Tr_Q \left\{ U_B^+(t) \, \Delta V \, U_B(t) \, \Delta V \, \rho_{eg} \right\} = \frac{1}{\hbar^2} \langle \Delta V(t) \Delta V(0) \rho_{eg} \rangle$$

We have $\boxed{C(-t) = C^*(t)}$

$$\langle \Delta V(-t) \Delta V(0) \rho_{eg} \rangle =$$
$$= \langle \Delta V^+(+t) \Delta V^+(0) \rho_{eg}^+ \rangle$$
$$= \langle \Delta V(t) \Delta V(0) \rho_{eg} \rangle^*$$

We can write (define)

real $\rightarrow$ $$C'(t) = \frac{1}{2\hbar^2} \left[\langle \Delta V(t) \Delta V(0) \rho_{eg} \rangle + \langle \Delta V(0) \Delta V(t) \rho_{eg} \rangle \right]$$

imaginary $\rightarrow$ $$C''(t) = -\frac{i}{2\hbar^2} \left[\langle \Delta V(t) \Delta V(0) \rho_{eg} \rangle - \langle \Delta V(0) \Delta V(t) \rho_{eg} \rangle \right]$$

$$\boxed{C(t) = C'(t) + i C''(t)}$$

also

$$\langle U_B(t) \Delta V \, U_B^+(t) \Delta V \rho_{eg} \rangle$$
$$= \langle \Delta V \, \Delta V(t) \rho_{eg} \rangle$$

Expansion into eigenstates

$$\boxed{C(t) = \frac{1}{\hbar^2} \sum_{ac} P(a) \, |V_{ac}|^2 \, e^{-i\omega_{ca} t}}$$

$$\Rightarrow \quad \boxed{C'(t) = \sum_{a,c} \frac{P(c) + P(a)}{2\hbar^2} \, |V_{ac}|^2 \cos(\omega_{ca} t)}$$

$$C''(t) = \sum_{ac} \frac{P(c) - P(a)}{2\hbar^2} |V_{ac}|^2 \sin \omega_{ac} t$$

It is useful to switch into frequency domain and introduce so-called spectral density

$$\tilde{C}(\omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} C(t) = 2 \mathrm{Re} \int_0^{\infty} dt \, e^{i\omega t} C(t)$$

thanks to its symmetry

$$\tilde{C}(\omega) = 2 \mathrm{Re} \int_0^{\infty} dt \, e^{i\omega t} \, C'(t) + i C''(t) =$$

$i \cos\omega t + i (i) \sin\omega t$

$$= 2 \mathrm{Re} \int_0^{\infty} dt \, e^{i\omega t} \, C'(t) + 2 \mathrm{Re} \, i \int_0^{\infty} dt \, e^{i\omega t} \, C''(t)$$

$$= 2 \int_0^{\infty} dt \cos\omega t \, C'(t) - 2 \int_0^{\infty} dt \sin\omega t \, C''(t)$$

We introduce ~~Zavedeme~~

$$\tilde{C}'(\omega) = 2 \int_0^{\infty} dt \cos\omega t \, C'(t)$$

$$\tilde{C}''(\omega) = -2 \int_0^{\infty} dt \sin\omega t \, C''(t)$$

Both are real and have properties $\tilde{C}'(\omega) = \tilde{C}'(-\omega)$

$\tilde{C}''(\omega) = -\tilde{C}''(-\omega)$

In eigenstates we can write

$$\tilde{C}(\omega) = \frac{2\pi}{\hbar^2} \sum_{ac} P(a) \, |V_{ac}|^2 \, \delta(\omega - \omega_{ca})$$

$$\tilde{C}'(\omega) = \frac{\pi}{\hbar^2} \sum_{ac} \left[P(a) + P(c)\right] |V_{ac}|^2 \, \delta(\omega - \omega_{ca})$$

$$\tilde{C}''(\omega) = \frac{\pi}{\hbar^2} \sum_{ac} \left[P(a) - P(c)\right] |V_{ac}|^2 \, \delta(\omega - \omega_{ca})$$

Because $P(a)$ is an equilibrium distribution of populations

$$\Rightarrow \quad \boxed{\tilde{C}(-\omega) = \exp(-\beta\hbar\omega) \, \tilde{C}(\omega)}$$

We can also derive

$$\tilde{C}'(\omega) = \frac{1 + e^{-\beta\hbar\omega}}{2} \, \tilde{C}(\omega)$$

$$\tilde{C}''(\omega) = \frac{1 - e^{-\beta\hbar\omega}}{2} \, \tilde{C}(\omega)$$

$$\Rightarrow \quad \boxed{\begin{aligned} \tilde{C}'(\omega) &= \coth(\beta\hbar\omega/2) \, \tilde{C}''(\omega) \\ \tilde{C}(\omega) &= \left[1 + \coth(\beta\hbar\omega/2)\right] \tilde{C}''(\omega) \end{aligned}}$$

$\Rightarrow$ $C'(t)$ and $C''(t)$ are not independent

Back to $C(t)$

$$C(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\, \tilde{C}'(\omega) + i\tilde{C}''(\omega) =$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} \coth(\beta\hbar\omega/2)\, \tilde{C}''(\omega)$$

$$+ \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\, \tilde{C}''(\omega)$$

Due to symmetries

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \cos(\omega t) \coth(\beta\hbar\omega/2)\, \tilde{C}''(\omega)$$

$$- \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\, \sin(\omega t)\, \tilde{C}''(\omega)$$

← this allows to express $C(t)$ in terms of $\tilde{C}'(t)$

One can also write

$$g(t) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{\tilde{C}(\omega)}{\omega^2}\left[e^{-i\omega t} + i\omega t - 1\right]$$

$$\Rightarrow g(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{1-\cos\omega t}{\omega^2} \coth(\beta\hbar\omega/2)\, \tilde{C}''(\omega)$$

$$+ \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{\sin\omega t - \omega t}{\omega^2}\, \tilde{C}''(\omega)$$

$$g(t) = \Delta^2 \int_0^t d\tau_2 \int_0^{\tau_2} d\tau_1 \, M'(\tau_1) - i\lambda \int_0^t d\tau \, [1 - M''(\tau)]$$

$$M'(t) = \frac{1}{\pi\Delta^2} \int_0^\infty d\omega \, \tilde{C}''(\omega) \coth(\beta\hbar\omega/2) \cos\omega t$$

$$M''(t) = \frac{1}{\pi\lambda} \int_0^\infty d\omega \, \frac{\tilde{C}''(\omega)}{\omega} \cos\omega t$$

$$\Delta^2 = \frac{1}{\pi} \int_0^\infty d\omega \, \tilde{C}''(\omega) \coth(\beta\hbar\omega/2)$$

$$\lambda = \frac{1}{\pi} \int_0^\infty d\omega \, \frac{\tilde{C}''(\omega)}{\omega}$$

Two parameters of the coupling Δ and λ

$$M'(t) = C'(t)/C'(t=0) \quad \Rightarrow M'(t=0) = 1 = M''(t=0)$$

$$\Delta^2 = C'(t=0)$$

real functions

For imaginary part we have

$$\int_0^t d\tau \, C''(\tau) \equiv \lambda[1 - M''(t)]$$

$$\lambda = \int_0^\infty dt \, C''(\tau)$$

$$\Rightarrow M''(t) = 1 - \int_0^t d\tau \, C''(\tau) \Big/ \int_0^\infty d\tau \, C''(\tau)$$

at high temperature

$$\beta\hbar\omega \ll 1 \Rightarrow \coth(\beta\hbar\omega/2) \approx \frac{2k_B T}{\hbar\omega}$$

$$\Rightarrow \Delta^2 = \frac{2\lambda k_B T}{\hbar}$$

$$M'(t) = M''(t) \equiv M(t)$$

$$g(t) = \frac{2\lambda k_B T}{\hbar} \int_0^t d\tau \int_0^{t_2} d\tau_1\, M(\tau_1) - i\lambda \int_0^t d\tau_2 \left[1 - M(\tau_2)\right]$$

$$M(t) = \frac{1}{\pi\lambda} \int_0^\infty d\omega\, \frac{\tilde{C}''(\omega)}{\omega} \cos(\omega t) \qquad \beta\hbar\omega \ll 1$$

$$\lambda = \frac{1}{\pi} \int_0^\infty d\omega\, \frac{\tilde{C}''(\omega)}{\omega}$$

Ansatz:

$$\tilde{C}''(\omega) = 2\lambda \frac{\omega\Lambda}{\omega^2 + \Lambda^2}$$