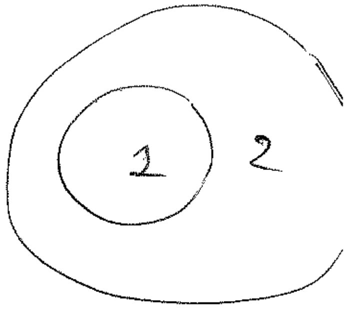
unit mass

GLE : classical & quantum

22.08.11

§1. Classical treatment

~~using $\mathcal{H}_2^0$ for averaging~~



1. Our Hamiltonian:

$$\mathcal{H} = \mathcal{H}_1 + \underbrace{\mathcal{H}_2^0 + \mathcal{H}_{12}}_{\mathcal{H}_2} \qquad (1)$$

$$\mathcal{H}_1 = \frac{1}{2} P_1^T P_1 + \mathcal{U}_1(X_1) \qquad (2)$$

$$\mathcal{H}_2^0 = \frac{1}{2} P_2^T P_2 + \frac{1}{2} X_2^T \mathcal{D}_{22} X_2 \quad , \quad \mathcal{H}_{12} = V_2^T(X_1)\, X_2 \leftarrow \text{interaction} \qquad (3)$$

2. Equations of motion:

$$\ddot{X}_1 = f_1 - V_{12} X_2 \quad , \quad \ddot{X}_2 = - V_2 - \mathcal{D}_{22} X_2 \qquad (4)(5)$$

with $f_1 = -\frac{\partial}{\partial X_1} \mathcal{U}_1(X_1)$, $V_{12} = \frac{\partial}{\partial X_1} V_2(X_1)$ (6)

3. Solving for X_2:

- If $\mathcal{D}_{22} e_{\lambda 2} = \omega_\lambda^2 e_{\lambda 2}$, then: (7)

$$X_2(t) = \dot{\Omega}_{22}(t,t_0)\, X_2(t_0) + \Omega_{22}(t,t_0) \overbrace{\dot{X}_2(t_0)}^{P_2(t_0)} - \int_{t_0}^{t} \Omega_{22}(t,\tau)\, V_2(\tau)\, d\tau \qquad (8)$$

where

$$\boxed{\Omega_{22}(t,t') = \sum_\lambda \frac{e_\lambda e_\lambda^T}{\omega_\lambda} \sin \omega_\lambda (t-t_0)} \qquad (9)$$

(we shall omit the index 2 in $e_{\lambda 2} \to e_\lambda$). Here $V_2(\tau)$ depends on τ via X_1: $V_2(\tau) \equiv V_2(X_1(\tau))$.

- Substitute $X_2(t)$ into the EoM for $X_1(t)$:

$$\ddot{X}_1 = f_1 - V_{12}(t)\left[\dot{\Omega}_{22}(t,t_0)\, X_2(t_0) + \Omega_{22}(t,t_0)\, P_2(t_0)\right] + \int_{t_0}^{t} d\tau\; V_{12}(t)\, \Omega_{22}(t,\tau)\, V_2(\tau)\, d\tau \qquad (10)$$

If we denote

$$\boxed{R_1(t) = - V_{12}(t)\left[\dot{\Omega}_{22}(t,t_0)\, X_2(t_0) + \Omega_{22}(t,t_0)\, P_2(t_0)\right]} \qquad (11)$$

$$\boxed{\ddot{X}_1 = f_1 + R_1 + \int_{t_0}^{t} d\tau\; V_{12}(t)\, \Omega_{22}(t,\tau)\, \underbrace{V_2(\tau)}_{\to\, V_2(X_1(\tau))}} \qquad \text{Form 1} \qquad (12)$$

This will be called the <u>Form 1</u> of GLE,

- To obtain <u>Form 2</u> of GLE, we take the integral by parts:

$$\int_{t_0}^{t} d\tau\, \Omega_{22}(t,\tau)\, V_2(X_1(\tau)) = \sum_\lambda \frac{e_\lambda e_\lambda^+}{\omega_\lambda} \int_{t_0}^{t} d\tau\, \sin\omega_\lambda(t-\tau)\, V_2(X_1(\tau))$$

$$= \sum_\lambda \frac{e_\lambda e_\lambda^+}{\omega_\lambda} \left\{ \frac{1}{\omega_\lambda}\cos\omega_\lambda(t-\tau)\, V_2(X_1(\tau)) \Big|_{t_0}^{t} - \int_{t_0} \frac{1}{\omega_\lambda}\cos\omega_\lambda(t-\tau)\, V_{21}(\tau)\, \underbrace{\dot{X}_1(\tau)}_{P_1(\tau)}\, d\tau \right\}$$

$$= \sum_\lambda \frac{e_\lambda e_\lambda^+}{\omega_\lambda^2} \left\{ V_2(t) - \cos\omega_\lambda(t-t_0)\, V_2(X_1(t_0)) - \int_{t_0}^{t} \cos\omega_\lambda(t-\tau)\, V_{21}(\tau)\, P_1(\tau)\, d\tau \right\}$$

$$= \mathcal{D}_{22}^{-1} V_2(t) - \Pi_{22}(t,t_0)\, V_2(t_0) - \int_{t_0}^{t} \Pi_{22}(t,\tau)\, V_{21}(\tau)\, P_1(\tau)\, d\tau \qquad (13)$$

where

$$\boxed{\Pi_{22}(t,t') = \sum_\lambda \frac{e_\lambda e_\lambda^+}{\omega_\lambda^2} \cos\omega_\lambda(t-t')} \qquad (14)$$

Substitute (13) in (10):

$$\ddot{X}_1 = \cancel{[f_1 + \mathcal{D}_{22}^{-1} V_2(t)]}\, f_1 + V_{12}(t)\,\mathcal{D}_{22}^{-1} V_2(t) - V_{12}(t)\, \Pi_{22}(t,t_0)\, V_2(t_0)$$

$$- V_{12}(t)\left[\dot{\Omega}_{22}(t,t_0)\, X_2(t_0) + \Omega_{22}(t,t_0)\, P_2(t_0)\right] - \int_{t_0}^{t} d\tau \left[V_{12}(t)\, \Pi_{22}(t,\tau)\, V_{21}(\tau)\right] P_1(\tau)$$

Denoting

$$\boxed{R_1(t) = -V_{12}(t)\left[\dot{\Omega}_{22}(t,t_0)\, X_2(t_0) + \Omega_{22}(t,t_0)\, P_2(t_0) + \Pi_{22}(t,t_0)\, V_2(t_0)\right]} \qquad (15)$$

$$\boxed{\Gamma_{11}(t,\tau) = V_{12}(t)\, \Pi_{22}(t,\tau)\, V_{21}(\tau)} \qquad (16)$$

~~we finally~~

$$\boxed{F_1(t) = f_1(t) + V_{12}(t)\, \mathcal{D}_{22}^{-1} V_2(t)} \qquad (17)$$

we obtain the other form of GLE:

$$\boxed{\ddot{X}_1 = F_1 + R_1 - \int_{t_0}^{t} d\tau\, \Gamma_{11}(t,\tau)\, P_1(\tau)} \qquad \text{Form 2} \qquad (18)$$

4. The force $R_1(t)$ in both forms depends on the initial conditions at t_0. Statistics wrt region 2 is required to study properties of $R_1(t)$. And the former depends on the Form 1 or 2 of GLE chosen.

(i) Form 1
$$\boxed{\rho_2^{eq} = \frac{1}{Z_2} e^{-\beta \mathcal{H}_2^0}} \qquad \text{(no interaction between regions)} \qquad (19)$$

• Normal coordinates $\xi_\lambda(t)$:

$$\mathcal{H}_2^0 = \frac{1}{2} P_2^T P_2 + \frac{1}{2} X_2^T \mathcal{D}_{22} X_2 \quad , \quad \boxed{\xi_\lambda = e_\lambda^\dagger X_2} \, , \, \boxed{\dot{\xi}_\lambda = e_\lambda^\dagger \dot{X}_2 = e_\lambda^\dagger P_2} \qquad (20)$$

so that
$$\boxed{X_2 = \sum_\lambda e_\lambda \xi_\lambda} \, , \quad \boxed{P_2 = \dot{X}_2 = \sum_\lambda e_\lambda \dot{\xi}_\lambda} \qquad (21)$$

$$KE = \frac{1}{2} P_2^T P_2 = \frac{1}{2} \sum_\lambda \dot{\xi}_\lambda e_\lambda^\dagger \sum_{\lambda'} \dot{\xi}_{\lambda'} e_{\lambda'} = \frac{1}{2} \sum_{\lambda\lambda'} \dot{\xi}_\lambda \dot{\xi}_{\lambda'} \underset{\overset{\shortparallel}{\delta_{\lambda\lambda'}}}{(e_\lambda^\dagger e_{\lambda'})} = \frac{1}{2} \sum_\lambda \dot{\xi}_\lambda^2$$

$$PE = \frac{1}{2} X_2^T \mathcal{D}_{22} X_2 = \frac{1}{2} \sum_{\lambda\lambda'} \xi_\lambda e_\lambda^\dagger \underbrace{\mathcal{D}_{22} e_{\lambda'}}_{\omega_{\lambda'}^2 e_{\lambda'}} \xi_{\lambda'} = \frac{1}{2} \sum_{\lambda\lambda'} \xi_\lambda \xi_{\lambda'} \omega_{\lambda'}^2 \underbrace{e_\lambda^\dagger e_{\lambda'}}_{\delta_{\lambda\lambda'}} = \frac{1}{2} \sum_\lambda \omega_\lambda^2 \xi_\lambda^2$$

so that
$$\boxed{\mathcal{H}_2^0 = \sum_\lambda \frac{1}{2} \left(\dot{\xi}_\lambda^2 + \omega_\lambda^2 \xi_\lambda^2 \right) = \sum_\lambda \mathcal{H}_\lambda^0} \qquad (22)$$

• Write the R_1-force:

$$R_1 = -V_{12} \left[\dot{\Omega}_{22}(t,t_0) X_2(t_0) + \Omega_{22}(t,t_0) P_2(t_0) \right]$$

$$= -V_{12} \left\{ \sum_\lambda e_\lambda e_\lambda^\dagger \cos\omega_\lambda (t-t_0) \cdot \sum_{\lambda'} e_{\lambda'} \xi_{\lambda'}(t_0) + \sum_\lambda \frac{e_\lambda e_\lambda^\dagger}{\omega_\lambda} \sin\omega_\lambda (t-t_0) \cdot \sum_{\lambda'} e_{\lambda'} \dot{\xi}_{\lambda'}(t_0) \right\}$$

$$= -V_{12} \sum_{\lambda\lambda'} \left\{ e_\lambda \underbrace{e_\lambda^\dagger e_{\lambda'}}_{\delta_{\lambda\lambda'}} \left[\cos\omega_\lambda (t-t_0) \, \xi_{\lambda'}(t_0) + \frac{\sin\omega_\lambda (t-t_0)}{\omega_\lambda} \dot{\xi}_{\lambda'}(t_0) \right] \right\}$$

$$= -V_{12} \sum_\lambda \left[\cos\omega_\lambda (t-t_0) \left(e_\lambda \xi_\lambda(t_0) \right) + \frac{\sin\omega_\lambda (t-t_0)}{\omega_\lambda} \left(e_\lambda \dot{\xi}_\lambda(t_0) \right) \right] \qquad (23)$$

It is linear in ξ_λ, $\dot{\xi}_\lambda$, so that

$$\langle R_1 \rangle_t = \int d\Gamma \, \rho_2^{eq} R_1(t) = 0 \qquad (24)$$

since

$$\langle \xi_\lambda \rangle_{t_0} = \int \{d\xi_\lambda\} \{d\dot{\xi}_\lambda\} \left(\prod_{\lambda'} \frac{1}{Z_{\lambda'}} e^{-\beta \mathcal{H}_{\lambda'}^0} \right) \xi_\lambda = \frac{1}{Z_\lambda^{(\xi)}} \int d\xi_\lambda \, e^{-\beta \frac{1}{2} \omega_\lambda^2 \xi_\lambda^2} \xi_\lambda = 0 \qquad (25)$$

$$\langle \dot{\xi}_\lambda \rangle_{t_0} = \frac{1}{Z_\lambda^{(\dot{\xi})}} \int d\dot{\xi}_\lambda \, e^{-\beta \frac{1}{2} \dot{\xi}_\lambda^2} \dot{\xi}_\lambda = 0 \quad \text{as well.} \qquad (26)$$

• $R_1(t)$ is a sum of Gaussian distributed quantities $\xi_\lambda(t_0)$ and $\dot{\xi}_\lambda(t_0)$, so that it is also Gaussian. Calculate the correlation function:

$$\langle R_1(t) R_1^T(t')\rangle = V_{12}(t)\Big\{ \dot{\Omega}_{22}(t,t_0) \langle X_2(t_0) X_2^T(t_0)\rangle \dot{\Omega}_{22}(t',t_0) +$$
$$+ \dot{\Omega}_{22}(t,t_0) \langle X_2(t_0) P_2^T(t_0)\rangle \Omega_{22}(t',t_0)$$
$$+ \Omega_{22}(t,t_0) \langle P_2(t_0) X_2^T(t_0)\rangle \dot{\Omega}_{22}(t',t_0)$$
$$+ \Omega_{22}(t,t_0) \langle P_2(t_0) P_2^T(t_0)\rangle \Omega_{22}(t',t_0) \Big\} V_{21}(t') \qquad (27)$$

We need to calculate all the correlation functions here. We shall start with the elementary ones:

$$\langle \xi_\lambda \xi_{\lambda'}\rangle = \cancel{\tfrac{1}{2}} \int d\Gamma\, \xi_\lambda \xi_{\lambda'} \frac{1}{Z} \prod_{\lambda_1} e^{-\beta \mathcal{H}_{\lambda_1}} = \delta_{\lambda\lambda'} \int d\xi_\lambda \frac{1}{Z_\lambda(\xi)} e^{-\beta \frac{\omega_\lambda^2}{2} \xi_\lambda^2} \xi_\lambda^2$$

Firstly,

$$Z_\lambda(\xi) = \int_{-\infty}^{\infty} d\xi_\lambda\, e^{-\beta \frac{1}{2}\omega_\lambda^2 \xi_\lambda^2} = \sqrt{\frac{\pi}{\beta \frac{1}{2}\omega_\lambda^2}} = \sqrt{\frac{2\pi}{\beta\omega_\lambda^2}}$$

Secondly,

$$\int d\xi_\lambda\, \xi_\lambda^2\, e^{-\left(\beta\frac{\omega_\lambda^2}{2}\right)\xi_\lambda^2} = \frac{\sqrt{\pi}}{2} \frac{1}{\left(\beta\frac{\omega_\lambda^2}{2}\right)\sqrt{\frac{\beta\omega_\lambda^2}{2}}} = \frac{\sqrt{\pi}}{2}\frac{2\sqrt{2}}{\beta\omega_\lambda^2\sqrt{\beta\omega_\lambda^2}} = \sqrt{\frac{2\pi}{\beta\omega_\lambda^2}}\cdot\frac{1}{\beta\omega_\lambda^2}$$

so that

$$\langle \xi_\lambda \xi_{\lambda'}\rangle = \delta_{\lambda\lambda'} \sqrt{\frac{\beta\omega_\lambda^2}{2\pi}} \cdot \sqrt{\frac{2\pi}{\beta\omega_\lambda^2}} \cdot \frac{1}{\beta\omega_\lambda^2} \equiv \frac{\delta_{\lambda\lambda'}}{\beta\omega_\lambda^2} \qquad (28)$$

$$\langle \xi_\lambda \dot{\xi}_{\lambda'}\rangle = 0 \qquad (29)$$

$$\langle \dot{\xi}_\lambda \dot{\xi}_{\lambda'}\rangle = \delta_{\lambda\lambda'} \int d\dot{\xi}_\lambda \frac{1}{Z_\lambda(\dot{\xi})} e^{-\beta\frac{1}{2}\dot{\xi}_\lambda^2}$$

Since $Z_\lambda(\dot{\xi}) = \int_{-\infty}^{\infty} d\dot{\xi}_\lambda\, e^{-\beta\frac{1}{2}\dot{\xi}_\lambda^2} = \sqrt{\frac{\pi}{\beta/2}} = \sqrt{\frac{2\pi}{\beta}}$,

then

$$\langle \dot{\xi}_\lambda \dot{\xi}_{\lambda'}\rangle = \delta_{\lambda\lambda'} \sqrt{\frac{\beta}{2\pi}} \cdot \frac{\sqrt{\pi}}{2} \frac{1}{\sqrt{\frac{\beta}{2}}\cdot\frac{\beta}{2}} = \delta_{\lambda\lambda'}\frac{1}{\beta} \qquad (30)$$

- These relations allows us to calculate the needed averages in Eq. (27):

$$\langle X_2 X_2^T\rangle = \sum_{\lambda\lambda'} e_\lambda \langle \xi_\lambda \xi_{\lambda'}\rangle e^+_{\lambda'} = \sum_\lambda e_\lambda e^+_\lambda \cdot \frac{1}{\beta\omega_\lambda^2} = \frac{1}{\beta} \mathcal{D}_{22}^{-1} \qquad (31)$$

$$\langle X_2 P_2^T\rangle = \sum_{\lambda\lambda'} e_\lambda \langle \xi_\lambda \dot{\xi}_{\lambda'}\rangle e^+_{\lambda'} = 0 \qquad (32)$$

$$\langle P_2 P_2^+\rangle = \sum_{\lambda\lambda'} e_\lambda \langle \dot{\xi}_\lambda \dot{\xi}_{\lambda'}\rangle e^+_{\lambda'} = \sum_\lambda e_\lambda e^+_\lambda \frac{1}{\beta} = \frac{1}{\beta} \mathbb{1}_{22} \qquad (33)$$

which allow us to rewrite (27) as follows:

$$\langle R_1(t) R_1^T(t')\rangle = V_{12}(t) \left\{ \dot{\Omega}_{22}(t,t_0) \frac{1}{\beta} \mathcal{D}_{22}^{-1} \dot{\Omega}_{22}(t',t_0) + \frac{1}{\beta} \Omega_{22}(t,t_0) \Omega_{22}(t',t_0)\right\} V_{21}(t')$$

$$= \frac{1}{\beta} V_{12}(t) \left\{ \dot{\Omega}_{22}(t,t_0) \cancel{\dot{\Omega}_{22}(t',t_0)} \mathcal{D}_{22}^{-1} \dot{\Omega}_{22}(t',t_0) + \Omega_{22}(t,t_0)\Omega_{22}(t',t_0)\right\} V_{21}(t')$$

The expression in the brackets:

$$\{\dots\} = \frac{1}{\beta}\Big(\sum_\lambda e_\lambda \overbrace{e^+_\lambda \cos\omega_\lambda(t-t_0)\Big)\Big(\sum_{\lambda'} e_{\lambda'}}^{\delta_{\lambda\lambda'}} \overbrace{e^+_{\lambda'} \omega_{\lambda'}^{-2}\Big)\Big(\sum_{\lambda''} e_{\lambda''}}^{\delta_{\lambda'\lambda''}} e^+_{\lambda''} \cos\omega_{\lambda''}(t'-t_0)\Big) +$$

$$+ \frac{1}{\beta}\Big(\sum_\lambda e_\lambda \overbrace{e^+_\lambda \frac{\sin\omega_\lambda(t-t_0)}{\omega_\lambda}\Big)\Big(\sum_{\lambda'} e_{\lambda'}}^{\delta_{\lambda\lambda'}} e^+_{\lambda'} \frac{\sin\omega_{\lambda'}(t'-t_0)}{\omega_{\lambda'}}\Big)$$

$$= \frac{1}{\beta}\sum_\lambda e_\lambda e^+_\lambda \left[\frac{1}{\omega_\lambda^2}\cos\omega_\lambda(t-t_0)\cos\omega_\lambda(t'-t_0) + \frac{1}{\omega_\lambda^2}\sin\omega_\lambda(t-t_0)\sin\omega_\lambda(t'-t_0)\right]$$

$$= \frac{1}{\beta}\sum_\lambda \frac{e_\lambda e^+_\lambda}{\omega_\lambda^2}\left[\cos\omega_\lambda(t-t_0)\cos\omega_\lambda(t'-t_0) + \sin\omega_\lambda(t-t_0)\sin\omega_\lambda(t'-t_0)\right]$$

$$= \frac{1}{\beta}\sum_\lambda \frac{e_\lambda e^+_\lambda}{\omega_\lambda^2}\cos\omega_\lambda(t-t') \equiv \frac{1}{\beta}\Pi_{22}(t,t') \qquad (34)$$

which gives:

$$\boxed{\langle R_1(t) R_1^T(t')\rangle = \frac{1}{\beta} V_{12}(t)\,\Pi_{22}(t,t')\,V_{21}(t') \equiv \frac{1}{\beta}\Gamma_{11}(t,t')} \qquad \text{Form 1} \quad (35)$$

In particular, at $t_0 = t'$,

$$\boxed{\langle R_1(t_0) R_1^T(t_0)\rangle = \frac{1}{\beta} V_{12}(t_0)\,\Pi_{22}(t,t)\,V_{21}(t) = \frac{1}{\beta} V_{12}(t)\,\mathcal{D}_{22}^{-1}\,V_{21}(t)} \qquad (36)$$

This is the dispersion at time t of the multivariable Gaussian describing $R_1(t)$ in the Stochastic GLE (12).

(ii) Form 2 $\qquad \rho_{eq} = \frac{1}{Z_2} e^{-\beta \mathcal{H}_2}$ (interaction is included!)

- Normal coordinates:

$$X_2 = \sum_\lambda e_\lambda \xi_\lambda \,, \quad \dot{X}_2 = P_2 = \sum_\lambda e_\lambda \dot{\xi}_\lambda$$

as before,

$$\mathcal{H}_2 = \frac{1}{2} P_2^T P_2 + \frac{1}{2} X_2^T \mathcal{D}_{22} X_2 + V_2^T X_2$$

$$KE = \frac{1}{2} P_2^T P_2 = \frac{1}{2} \sum_\lambda \dot{\xi}_\lambda^2$$

$$PE^{(1)} = \frac{1}{2} X_2^T \mathcal{D}_{22} X_2 = \frac{1}{2} \sum_\lambda \omega_\lambda^2 \xi_\lambda^2$$

as before, and

as e_λ are real!

$$PE^{(2)} = V_2^T X_2 = V_2^T \sum_\lambda e_\lambda \xi_\lambda = \sum_\lambda V_\lambda \xi_\lambda \,, \quad \boxed{V_\lambda = e_\lambda^{+} V_2} \qquad (37)$$

so that

$$\boxed{\mathcal{H}_2 = \sum_\lambda \mathcal{H}_\lambda \,, \quad \mathcal{H}_\lambda = \frac{1}{2}\left(\dot{\xi}_\lambda^2 + \omega_\lambda^2 \xi_\lambda^2\right) + V_\lambda \xi_\lambda} \qquad (38)$$

- Write the R_1-force ~~(15)~~ as in (15). We need the following elementary averages:

$$\langle \xi_\lambda\rangle = \int d\Gamma\, \xi_\lambda \frac{1}{Z} e^{-\beta \mathcal{H}_2} = \frac{1}{Z_\lambda(\xi)} \int d\xi_\lambda \cdot \xi_\lambda\, e^{-\beta\left[\frac{1}{2}\omega_\lambda^2 \xi_\lambda^2 + V_\lambda \xi_\lambda\right]}$$

$$\langle \dot{\xi}_\lambda\rangle = \frac{1}{Z_\lambda(\dot{\xi}_\lambda)} \int d\dot{\xi}_\lambda\, \dot{\xi}_\lambda\, e^{-\beta \frac{1}{2} \dot{\xi}_\lambda^2} = 0$$

Here

$$Z_\lambda(\xi) = \int_{-\infty}^{\infty} d\xi_\lambda\, e^{-\beta\left[\frac{1}{2}\omega_\lambda^2 \xi_\lambda^2 + V_\lambda \xi_\lambda\right]} = \int d\xi_\lambda\, e^{-\beta\left[\frac{1}{2}\omega_\lambda^2\left(\xi_\lambda + \frac{V_\lambda}{\omega_\lambda^2}\right)^2 - \frac{V_\lambda^2}{2\omega_\lambda^2}\right]}$$

$$= e^{\frac{\beta V_\lambda^2}{2\omega_\lambda^2}} \int dx\, e^{-\beta\frac{\omega_\lambda^2}{2}x^2} = e^{\frac{\beta V_\lambda^2}{2\omega_\lambda^2}} \sqrt{\frac{\pi}{\frac{\beta\omega_\lambda^2}{2}}} = e^{\frac{\beta V_\lambda^2}{2\omega_\lambda^2}} \sqrt{\frac{2\pi}{\beta\omega_\lambda^2}} , \quad (39)$$

$Z_\lambda(\mathring{\xi}) = \sqrt{\frac{2\pi}{\beta}}$ as before,

Now, we can calculate

$$\langle \xi_\lambda \rangle = \cancel{e^{-\beta V_\lambda^2/2\omega_\lambda^2}} \sqrt{\frac{\beta\omega_\lambda^2}{2\pi}} \cdot \int d\xi_\lambda \cdot \xi_\lambda \cancel{e^{\frac{\beta V_\lambda^2}{2\omega_\lambda^2}}}\, e^{-\beta\frac{1}{2}\omega_\lambda^2\left(\xi_\lambda + \frac{V_\lambda}{\omega_\lambda^2}\right)^2}$$

$$= \sqrt{\frac{\beta\omega_\lambda^2}{2\pi}} \cdot \int d\xi_\lambda \Big[\underbrace{\left(\xi_\lambda + \frac{V_\lambda}{\omega_\lambda^2}\right)}_{0} - \frac{V_\lambda}{\omega_\lambda^2} \Big] e^{-\beta\frac{\omega_\lambda^2}{2}\left(\xi_\lambda + \frac{V_\lambda}{\omega_\lambda^2}\right)^2}$$

$$= \sqrt{\frac{\beta\omega_\lambda^2}{2\pi}} \cdot \left(-\frac{V_\lambda}{\omega_\lambda^2}\right) \int_{-\infty}^{\infty} dx\, e^{-\beta\frac{\omega_\lambda^2}{2}x^2} = -\frac{V_\lambda}{\omega_\lambda^2} \quad (40)$$

so that

$$\langle X_2(t_0)\rangle = \sum_\lambda e_\lambda \langle \xi_\lambda \rangle = -\sum_\lambda \frac{e_\lambda V_\lambda}{\omega_\lambda^2}$$

As $V_\lambda = e_\lambda^\dagger V_2$ (see (37)), then

$$\cancel{\sum_\lambda e_\lambda^\dagger V_\lambda = V_2}$$

$$\langle X_2(t_0)\rangle = -\sum_\lambda \frac{e_\lambda}{\omega_\lambda^2} e_\lambda^\dagger V_2 = -\left(\sum_\lambda \frac{e_\lambda e_\lambda^\dagger}{\omega_\lambda^2}\right) V_2 = -\mathcal{D}_{22}^{-1} V_2(t_0) \quad (41)$$

~~Therefore,~~
Also,

$$\langle p_2(t_0)\rangle = \sum_\lambda e_\lambda \langle \mathring{\xi}_\lambda \rangle = 0 \quad (42)$$

Therefore, from (15):

$$\langle R_1(t)\rangle = -V_{12}(t)\left\{ \mathring{\Omega}_{22}(t,t_0)\langle X_2(t_0)\rangle + \Omega_{22}(t,t_0)\langle p_2(t_0)\rangle + \Pi_{22}(t,t_0)V_2(t_0) \right\}$$

$$= -V_{12}\left\{ -\mathring{\Omega}_{22}(t,t_0)\mathcal{D}_{22}^{-1}V_2(t_0) + \Pi_{22}(t,t_0)V_2(t_0)\right\}$$

$$= -V_{12}\left\{ -\mathring{\Omega}_{22}(t,t_0)\mathcal{D}_{22}^{-1} + \Pi_{22}(t,t_0)\right\} V_2(t_0)$$

Here

$$\{\ldots\} = \underbrace{-\Big(\sum_\lambda e_\lambda \overbrace{e_\lambda^\dagger \cos\omega_\lambda(t-t_0)\Big)\Big(\sum_{\lambda'} e_{\lambda'}}^{\delta_{\lambda\lambda'}} e_{\lambda'}^\dagger \omega_{\lambda'}^{-2}\Big)}_{-\sum_\lambda e_\lambda e_\lambda^\dagger \frac{\cos\omega_\lambda(t-t_0)}{\omega_\lambda^2} \equiv \Pi_{22}(t,t_0)} + \sum_\lambda \frac{e_\lambda e_\lambda^\dagger}{\omega_\lambda^2}\cos\omega_\lambda(t-t_0) \equiv 0$$

so, we have:

$$\boxed{\langle R_1(t)\rangle = 0} \qquad (43)$$

- We also calculate the correlation function:

$$\langle R_1(t) R_1^T(t')\rangle = V_{12}(t)\Big\{\mathring{\Omega}_{22}(t,t_0)\langle X_2 X_2^T\rangle \mathring{\Omega}_{22}(t',t_0) +$$

$$+ \mathring{\Omega}_{22}(t,t_0)\langle X_2 P_2^T\rangle \Omega_{22}(t',t_0) + \Omega_{22}(t,t_0)\langle P_2 X_2^T\rangle \mathring{\Omega}_{22}(t',t_0)$$

$$+ \Omega_{22}(t,t_0)\langle P_2 P_2^T\rangle \Omega_{22}(t',t_0) + \big(\cancel{\text{terms linear}}$$

$$+ \mathring{\Omega}_{22}(t,t_0)\langle X_2\rangle V_2^T(t_0)\Pi_{22}(t',t_0)$$

$$+ \Pi_{22}(t,t_0)V_2(t_0)\langle X_2^T\rangle \mathring{\Omega}_{22}(t',t_0) + (\text{terms linear in } \langle P_2\rangle \text{ are all zero})$$

$$+ \Pi_{22}(t,t_0)V_2(t_0)V_2^T(t_0)\Pi_{22}(t',t_0)\Big\} V_{21}(t') \qquad (44)$$

- Hence, we need elementary averages:

$$\langle X_2 X_2^T\rangle = \sum_{\lambda\lambda'} e_\lambda \langle \xi_\lambda \xi_{\lambda'}^*\rangle e_{\lambda'}^\dagger$$

where $\bar\xi_\lambda = \langle \xi_\lambda\rangle = -V_\lambda/\omega_\lambda^2$ (see (40)):

$$\langle \xi_\lambda \xi_{\lambda'}\rangle = \underbrace{\langle(\xi_\lambda - \bar\xi_\lambda)(\xi_{\lambda'} - \bar\xi_{\lambda'})\rangle}_{\sim\delta_{\lambda\lambda'}} + \bar\xi_\lambda \cdot \bar\xi_{\lambda'}$$

$$= \delta_{\lambda\lambda'}\langle(\xi_\lambda - \bar\xi_\lambda)^2\rangle + \frac{V_\lambda V_{\lambda'}}{\omega_\lambda^2 \omega_{\lambda'}^2},$$

$$\langle(\xi_\lambda - \bar\xi_\lambda)^2\rangle = \frac{1}{Z_\lambda(\xi)}\int_{-\infty}^{\infty} d\xi_\lambda (\xi_\lambda - \bar\xi_\lambda)^2 e^{-\beta\left[\frac{1}{2}\omega_\lambda(\xi_\lambda - \bar\xi_\lambda)^2 - \frac{V_\lambda^2}{2\omega_\lambda^2}\right]}$$

$$= \cancel{e^{-\frac{\beta V_\lambda^2}{2\omega_\lambda^2}}} \sqrt{\frac{\beta\omega_\lambda^2}{2\pi}} \cancel{e^{+\frac{\beta V_\lambda^2}{2\omega_\lambda^2}}} \cdot \frac{\sqrt{\pi}}{\cancel{2}} \frac{1}{\frac{\beta\omega_\lambda^2}{\cancel{2}}\sqrt{\frac{\beta\omega_\lambda^2}{2}}} = \frac{1}{\beta\omega_\lambda^2}$$

so that

$$\langle \xi_\lambda \xi_{\lambda'} \rangle = \frac{\delta_{\lambda\lambda'}}{\beta\omega_\lambda^2} + \frac{V_\lambda V_{\lambda'}}{\omega_\lambda^2 \omega_{\lambda'}^2} \tag{45}$$

and hence (see (41)):

$$\langle X_2 X_2^T \rangle = \sum_\lambda \frac{e_\lambda e_\lambda^\dagger}{\omega_\lambda^2} \beta^{-1} + \sum_\lambda \frac{e_\lambda V_\lambda}{\omega_\lambda^2} \sum_{\lambda'} \frac{V_{\lambda'} e_{\lambda'}^\dagger}{\omega_{\lambda'}^2}$$

$$= \mathcal{D}_{22}^{-1} \frac{1}{\beta} + \left(\mathcal{D}_{22}^{-1} V_2(t_0)\right)\left(V_2^T(t_0)\mathcal{D}_{22}^{-1}\right) \tag{46}$$

- $\langle X_2 P_2^T \rangle = \sum_{\lambda\lambda'} e_\lambda \langle \xi_\lambda \dot{\xi}_{\lambda'} \rangle e_{\lambda'}^\dagger$

$$\langle \xi_\lambda \dot{\xi}_{\lambda'} \rangle = \langle (\xi_\lambda - \bar{\xi}_\lambda)\dot{\xi}_{\lambda'} + \bar{\xi}_\lambda \dot{\xi}_{\lambda'} \rangle = \underbrace{\langle (\xi_\lambda - \bar{\xi}_\lambda)\dot{\xi}_{\lambda'} \rangle}_{=0} + \bar{\xi}_\lambda \underbrace{\langle \dot{\xi}_{\lambda'} \rangle}_{=0} = 0$$

$$\hookrightarrow \langle X_2 P_2^T \rangle = 0, \quad \langle P_2 X_2^T \rangle = 0 \tag{47}$$

- $\langle P_2 P_2^T \rangle = \sum_\lambda e_\lambda \langle \dot{\xi}_\lambda \dot{\xi}_{\lambda'} \rangle e_{\lambda'}^\dagger = \frac{1}{\beta} 1\!\!1_{22}$ since

$\langle \dot{\xi}_\lambda \dot{\xi}_{\lambda'} \rangle = \delta_{\lambda\lambda'} \frac{1}{\beta}$ as before, see (30).

- Now we can collect all terms in (44):

$$\langle R_1(t) R_1^T(t') \rangle = V_{12}(t) \Big\{ \dot{\Omega}_{22}(t,t_0) \left[\frac{1}{\beta}\mathcal{D}_{22}^{-1} + \left(\mathcal{D}_{22}^{-1} V_2(t_0)\right)\left(V_2^T(t_0)\mathcal{D}_{22}^{-1}\right)\right] \dot{\Omega}_{22}(t',t_0)$$

$$+ \Omega_{22}(t,t_0)\frac{1}{\beta}\Omega_{22}(t',t_0) - \dot{\Omega}_{22}(t,t_0)\mathcal{D}_{22}^{-1} V_2(t_0) V_2^T(t_0) \Pi_{22}(t',t_0)$$

$$- \Pi_{22}(t,t_0) V_2(t_0) V_2^T(t_0) \mathcal{D}_{22}^{-1} \dot{\Omega}_{22}(t',t_0) + \Pi_{22}(t,t_0) V_2(t_0) V_2^T(t_0) \Pi_{22}(t',t_0) \Big\} V_{21}(t') \tag{48}$$

Here:

$$\dot{\Omega}_{22}(t,t_0)\mathcal{D}_{22}^{-1}\dot{\Omega}_{22}(t',t_0) + \Omega_{22}(t,t_0)\Omega_{22}(t',t_0) = \frac{1}{\beta}\Pi_{22}(t,t') \tag{49}$$

$$\dot{\Omega}_{22}(t,t_0)\mathcal{D}_{22}^{-1} = \sum_\lambda e_\lambda \underbrace{e_\lambda^\dagger \cos\omega_\lambda(t-t_0) \sum_{\lambda'} e_{\lambda'}}_{\delta_{\lambda\lambda'}} e_{\lambda'}^\dagger \omega_{\lambda'}^{-2} = \Pi_{22}(t,t_0) \tag{50}$$

so that

$$\langle R_1(t) R_1^T(t') \rangle = V_{12}(t) \Big\{ \frac{1}{\beta} \Pi_{22}(t,t') + \Pi_{22}(t,t_0) V_2(t_0) V_2^T(t_0) \Pi_{22}(t',t_0)$$

$$- \Pi_{22}(t,t_0) V_2(t_0) V_2^T(t_0) \Pi_{22}(t',t_0) - \Pi_{22}(t,t_0) V_2(t_0) V_2^T(t_0) \Pi_{22}(t',t_0)$$

$$+ \Pi_{22}(t,t_0) V_2(t_0) V_2^T(t_0) \Pi_{22}(t',t_0) \Big\} V_{21}(t') \equiv \frac{1}{\beta} V_{12}(t) \Pi_{22}(t,t') V_{21}(t')$$

i.e. we obtain the same result as for the form 1:

$$\boxed{\langle R_1(t) R_1^T(t') \rangle = \frac{1}{\beta} \Gamma_{11}(t,t')} \qquad \text{(form 2)} \tag{51}$$

The dispersion $(t=t')$:

$$\langle R_1(t) R_1^T(t) \rangle = \frac{1}{\beta} \Gamma_{11}(t,t) = \frac{1}{\beta} V_{12}(t) \mathcal{D}_{22}^{-1} V_{21}(t) \tag{52}$$

as for the form 1.