22 April 08

§6. Thermal equilibrium

1. Similar to the Adelman & Doll paper, it is possible to consider thermal equilibrium at $t \to \infty$ limit.
We assume that after the thermodyn. process in question (e.g. ion bombardment upon the surface) the system would cool down and would become harmonic.
At $t = t_0 \to$ region 1 can be considered as harmonic. We would like to prove that at $t \gg t_0$ it would become canonical at the same T as of region 2 (the thermostat).

EOM:

$$M_1 \ddot{r}_1 = \tilde{f}_1 + R_1 - \int_0^t \Gamma_{11}(t-\tau)\dot{r}_1(\tau)\,d\tau$$

The integral:

$$\int_0^t \equiv \underbrace{\int_0^{t_0} \Gamma_{11}(t-\tau)\dot{r}_1(\tau)\,d\tau}_{\text{is small due to fast decrease of the friction kernel}} + \int_{t_0}^{t} \Gamma_{11}(t-\tau)\dot{r}_1(\tau)\,d\tau \simeq$$

$$\simeq \int_{t_0}^{t} \Gamma_{11}(t-\tau)\dot{r}_1(\tau)\,d\tau$$

Change (move) time, $t' = t - t_0$, gives EOM for t' (but we use t again for convenience):

$$\boxed{M_1 \ddot{r}_1 = \tilde{f}_1 + R_1 - \int_0^t \Gamma_{11}(t-\tau)\dot{r}_1(\tau)\,d\tau}$$

2. Due to harmonicity of region 1: (i) $r_1 \to u_1(t)$ (displacements)

(ii) $\tilde{f}_1 = f_1 + V_{12} D_{22}^{-1} V_2(t)$

with $f_1 \equiv -\Phi_{11} u_1$

(iii) $V_{12} \to \cancel{M_{12}}\ \Phi_{12} M_2^{-1/2}$, $V_2 \to M_2^{-1/2}\Phi_{21} u_1$

$\cancel{(IV)\ \Gamma_{11}(t) = V_{12}\,\Pi_{22}(t)\,V_{21}}$

~~Therefore~~

$$\cancel{V_{12}D_{22}^{-1}V_{2} = \Phi_{12}M_2^{-1/2}D_{22}^{-1}M_2^{-1/2}\Phi_{21}u_1 \equiv \Phi_{12}\Phi_{22}^{-1}\Phi_{21}u_1}$$

and $\cancel{\tilde{f}_1 = -D_{11}u_1 + \Phi_{12}\Phi_{22}^{-1}\Phi_{21}}$

$$V_{12} = \Phi_{12}M_2^{-1/2} = M_1^{1/2}M_1^{-1/2}\Phi_{12}M_2^{-1/2} = M_1^{1/2}D_{12}$$

$$V_2 = M_2^{-1/2}\Phi_{21}u_1 = \left(M_2^{-1/2}\Phi_{21}M_1^{-1/2}\right)\left(M_1^{1/2}u_1\right) = D_{21}\left(M_1^{1/2}u_1\right)$$

and also

$$f_1 \equiv -M_1^{1/2}\left(M_1^{-1/2}\Phi_{11}M_1^{-1/2}\right)\left(M_1^{1/2}u_1\right) \equiv -M_1^{1/2}D_{11}\left(M_1^{1/2}u_1\right)$$

so that

$$\tilde{f}_1 = -M_1^{1/2}\left[D_{11} - D_{12}D_{22}^{-1}D_{21}\right]\left(M_1^{1/2}u_1\right)$$

$$= -M_1^{1/2}\,\tilde{D}_{11}\left(M_1^{1/2}u_1\right)$$

Next, the friction kernel:

$$\Gamma_{11}(t) = V_{12}\,\Pi_{22}(t)\,V_{21} = M_1^{1/2}\left(D_{12}\,\Pi_{22}(t)\,D_{21}\right)M_1^{1/2}$$

$$\int_0^t \Gamma_{11}(t-\tau)\,\dot{u}_1(\tau)\,d\tau \equiv M_1^{1/2}\int_0^t \left(D_{12}\,\Pi_{22}(t-\tau)\,D_{21}\right)\left(M_1^{1/2}\dot{u}_1(\tau)\right)d\tau$$

We now introduce $\boxed{X_1 \equiv M_1^{1/2}u_1}$

<u>EOM:</u>

$$M_1^{1/2}\ddot{X}_1 = -M_1^{1/2}\tilde{D}_{11}X_1 + R_1 - M_1^{1/2}\int_0^t\left(D_{12}\,\Pi_{22}(t-\tau)\,D_{21}\right)\dot{X}_1(\tau)\,d\tau$$

$$\boxed{\ddot{X}_1 + \tilde{D}_{11}X_1 = \tilde{R}_1 - \int_0^t \tilde{\Gamma}_{11}(t-\tau)\,\dot{X}_1(\tau)\,d\tau},\qquad \boxed{\begin{array}{c}\tilde{R}_1 = M_1^{-1/2}R_1\\ \hline \tilde{\Gamma}_{11}(t) = D_{12}\,\Pi_{22}(t)\,D_{21}\end{array}}$$

Here:

$$\langle \tilde{R}_1 \rangle = 0$$

$$\langle \tilde{R}_1(t)\,\tilde{R}_1^{+}(t') \rangle = M_1^{-1/2}\langle R_1(t)\,R_1^{+}(t')\rangle M_1^{-1/2} =$$

$$= M_1^{-1/2}\frac{1}{\beta}\left[V_{12}\,\Pi_{22}(t-t')\,V_{21}\right]M_2^{-1/2} = \frac{1}{\beta}D_{12}\,\Pi_{22}(t-t')\,D_{21}$$

$$= \frac{1}{\beta}\tilde{\Gamma}_{11}(t-t')$$

$$\boxed{\tilde{\Gamma}_{11}(t-t') = \beta\ \langle \tilde{R}_1(t)\,\tilde{R}_1^{+}(t')\rangle}$$

We have the following properties of the kernel (and thus of the correl. function):

$$\tilde{\Gamma}_{ii'}(t-t') = \sum_{jj'\in 2} D_{ij}\,\Pi_{jj'}(t-t')\,D_{j'i'} \equiv \tilde{\Gamma}_{ii'}(t'-t)$$

$$\Pi_{jj'}(t) = \sum_\lambda \frac{e_{\lambda j}\,e_{\lambda j'}}{\omega_\lambda^2}\cos\omega_\lambda t \equiv \Pi_{j'j}(t)$$

~~Therefore,~~ Also:

$$\tilde{\Gamma}_{i'i}(t) = \sum_{jj'} D_{i'j}\,\Pi_{jj'}(t)\,D_{j'i} = \sum_{jj'} D_{ij'}\,\Pi_{j'j}\,D_{ji'} =$$

$$= \sum_{jj'} D_{ij'}\,\Pi_{j'j}\,D_{ji'} \equiv \tilde{\Gamma}_{ii'}(t),$$

i.e.

$$\boxed{\tilde{\Gamma}_{ii'}(t-t') = \tilde{\Gamma}_{ii'}(t'-t) = \tilde{\Gamma}_{i'i}(t-t')}$$

4. Now we solve eq. for $x_1(t)$. The method is the same as in Adelman & Doll (in fact, as in Adelman, ~~PRB~~ JCP 64 (1976) 124).

(i) do LS:

$$s^2 X_1(s) - sX_1(0) - \dot{X}_1(0) + \tilde{D}_{11}X_1(s) = \tilde{R}_1(s) - \tilde{\Gamma}_{11}(s)\left(sX_1(s) - X_1(0)\right)$$

$$\left[s^2\mathbb{1} + \tilde{D}_{11} + s\tilde{\Gamma}_{11}(s)\right]X_1(s) = \tilde{R}_1(s) + \left(s\mathbb{1} + \tilde{\Gamma}_{11}(s)\right)X_1(0) + \dot{X}_1(0)$$

If

$$\boxed{\begin{aligned} \chi_{11}(t) &= \mathcal{L}^{-1}(\chi_{11}(s)) \\ \chi_{11}(s) &= \left[s^2\mathbb{1} + \tilde{D}_{11} + s\tilde{\Gamma}_{11}(s)\right]^{-1} \end{aligned}}$$

Then,

$$X_1(s) = \mathcal{X}_{11}(s)\tilde{R}_1(s) + \mathcal{X}_{11}(s)(s\mathbb{1}_{11}+\tilde{\Gamma}_{11}(s))X_1(0) + \mathcal{X}_{11}(s)\dot{X}_1(0)$$

$\hookrightarrow$ $$\boxed{X_1(t) = \int_0^t \mathcal{X}_{11}(t-\tau)\tilde{R}_1(\tau)d\tau + \xi_{11}(t)X_1(0) + \mathcal{X}_{11}(t)\dot{X}_1(0)}$$

Here: $\xi_{11}(t) = \mathcal{L}^{-1}[\mathcal{X}_{11}(s)(s\mathbb{1}_{11}+\tilde{\Gamma}_{11}(s))]$,

and $\mathcal{X}_{11}(s\mathbb{1}_{11}+\tilde{\Gamma}_{11}) = (s^2\mathbb{1}_{11}+\tilde{D}_{11}+s\tilde{\Gamma}_{11})^{-1}(s\mathbb{1}_{11}+\tilde{\Gamma}_{11})$

$$= (s^2\mathbb{1}_{11}+\tilde{D}_{11}+s\tilde{\Gamma}_{11})^{-1}\left(s(s\mathbb{1}_{11}+\tilde{\Gamma}_{11})+\tilde{D}_{11}-\tilde{D}_{11}\right)\frac{1}{s}$$

$$= \frac{1}{s}\mathcal{X}_{11}\cdot(\mathcal{X}_{11}^{-1}-\tilde{D}_{11}) = \frac{1}{s} - \frac{1}{s}\mathcal{X}_{11}\tilde{D}_{11},$$

i.e.: $$\boxed{\xi_{11}(t) = 1 - \int_0^t \mathcal{X}_{11}(\tau)d\tau\cdot\tilde{D}_{11}} \Rightarrow \boxed{\dot{\xi}_{11}(t) = -\mathcal{X}_{11}(t)\tilde{D}_{11}}$$

We also see:

$$X_1(0) = \xi_{11}(0)X_1(0) + \mathcal{X}_{11}(0)\dot{X}_1(0) \rightarrow \boxed{\begin{matrix}\mathcal{X}_{11}(0)=0\\ \xi_{11}(0)=1\end{matrix}}$$

(the 2nd is consistent with $\xi_{11}(t)$ above).

Therefore, $$\boxed{\mathcal{L}[\dot{\mathcal{X}}_{11}(t)] = s\,\mathcal{X}_{11}(s)}$$

(ii) Next, we see that $X_1(t)$ is proportional to $\tilde{R}_1(\tau)$, i.e. it is a Gaussian process.

(iv) We also consider the velocities:

$$V_1(t) = \dot{R}_1(t) = \dot{u}_1(t)$$

$$X_1(t) = \sqrt{M_1}\,u_1(t) \rightarrow \boxed{v_1(t) = \sqrt{M_1}\,V_1(t) \equiv \dot{X}_1(t)}$$

$$v_1(t) = \int_0^t \dot{\mathcal{X}}_{11}(t-\tau)\tilde{R}_1(\tau)d\tau + \underbrace{\mathcal{X}_{11}(0)}_{=0}\tilde{R}_1(t) + \dot{\xi}_{11}(t)X_1(0) + \dot{\mathcal{X}}_{11}(t)\dot{X}_1(0)$$

$$v_1(t) = \dot{\xi}_{11}(t)\, x_1(0) + \mathring{\chi}_{11}(t)\, \dot{x}_1(0) + \int_0^t \mathring{\chi}_{11}(t-\tau)\, \tilde{R}_1(\tau)\, d\tau$$

where $\boxed{\dot{\xi}_{11}(t) = -\, \chi_{11}(t)\, \tilde{D}_{11}}$

so that, finally,

$$\boxed{v_1(t) = -\, \chi_{11}(t)\, \tilde{D}_{11}\, x_1(0) + \mathring{\chi}_{11}(t)\, \dot{x}_1(0) + \int_0^t \mathring{\chi}_{11}(t-\tau)\, \tilde{R}_1(\tau)\, d\tau}$$

(V) Relation to correlation functions (averaging wrt region 2):

$$\langle x_1(t)\, x_1^\dagger(0)\rangle = \xi_{11}(t)\, \langle x_1(0)\, x_1^\dagger(0)\rangle + \chi_{11}(t)\, \underbrace{\langle x_1(0)\, \dot{x}_1(0)\rangle}_{= 0}$$

(uncorrelated!)

↳ $\boxed{\xi_{11}(t) \sim \langle x_1(t)\, x_1^\dagger(0)\rangle}$

and thus should decay to zero as $t \to \infty$.

Similarly,

$$\langle x_1(t)\, v_1^\dagger(0)\rangle = \langle x_1(t)\, \dot{x}_1^\dagger(0)\rangle = \chi_{11}(t)\, \langle \dot{x}_1(0)\, \dot{x}_1^\dagger(0)\rangle,$$

so

$$\boxed{\chi_{11}(t) \sim \langle x_1(t)\, \dot{x}_1^\dagger(0)\rangle}$$

and should also decay to zero at $t \to \infty$.

(VI) Consider

$$y_1(t) = x_1(t) - \xi_{11}(t)\, x_1(0) - \chi_{11}(t)\, \dot{x}_1(0) \equiv \int_0^t \chi_{11}(t-\tau)\, \tilde{R}_1(\tau)\, d\tau$$

$$y_2(t) = \dot{x}_1(t) - \dot{\xi}_{11}(t)\, x_1(0) - \mathring{\chi}_{11}(t)\, \dot{x}_1(0) \equiv \int_0^t \mathring{\chi}_{11}(t-\tau)\, \tilde{R}_1(\tau)\, d\tau$$

and let us calculate their correlation functions at equal times:

$$A_{11} = \langle y_1(t)\, y_1^\dagger(t)\rangle = \int_0^t d\tau \int_0^t d\tau'\, \chi_{11}(t-\tau)\, \langle \tilde{R}_1(\tau)\, \tilde{R}_1^\dagger(\tau')\rangle\, \chi_{11}^\dagger(t-\tau')$$

$$= \int_0^t d\tau \int_0^t d\tau'\, \chi_{11}(t-\tau)\, \frac{1}{\beta}\, \tilde{\Gamma}_{11}(\tau-\tau')\, \chi_{11}^\dagger(t-\tau') =$$

$$= \left| \begin{matrix} t_1 = t-\tau \\ t_2 = t-\tau' \end{matrix} \right| = \frac{1}{\beta}\int_t^0 (-dt_1) \int_t^0 (-dt_2)\, \chi_{11}(t_1)\,\tilde\Gamma_{11}(t_2-t_1)\,\chi^\dagger_{11}(t_2)$$

$$\equiv \frac{1}{\beta}\int_0^t d\tau \int_0^t d\tau'\, \chi_{11}(\tau)\,\tilde\Gamma_{11}(\tau-\tau')\,\chi^\dagger_{11}(\tau')$$

since $\tilde\Gamma_{11}(\tau-\tau') = \tilde\Gamma_{11}(\tau'-\tau)$. Similarly:

$$A_{12} = \langle y_1(t)\, y_2^\dagger(t)\rangle = \frac{1}{\beta}\int_0^t d\tau \int_0^t d\tau'\, \chi_{11}(\tau)\,\tilde\Gamma_{11}(\tau-\tau')\,\dot\chi^\dagger_{11}(\tau')$$

$$A_{22} = \langle y_2(t)\, y_2^\dagger(t)\rangle = \frac{1}{\beta}\int_0^t d\tau \int_0^t d\tau'\, \dot\chi_{11}(\tau)\,\tilde\Gamma_{11}(\tau-\tau')\,\dot\chi^\dagger_{11}(\tau')$$

- Let us calculate

$$\cancel{A_{11}(t) = \frac{1}{\beta}\int_0^t d\tau\, \chi_{11}(\tau)\, \mathcal{L}^{-1}[\tilde\Gamma_{11}(s)\chi^\dagger_{11}(s)]},$$

$$\cancel{\tilde\Gamma_{11}(s)\chi^\dagger_{11}(s)} \quad \dot A_{11}(t) = \frac{1}{\beta}\chi_{11}(t)\int_0^t d\tau'\, \tilde\Gamma_{11}(t-\tau')\,\chi^\dagger_{11}(\tau') +$$

$$+ \frac{1}{\beta}\int_0^t d\tau\, \chi_{11}(\tau)\,\underbrace{\tilde\Gamma_{11}(\tau-t)}_{\equiv \tilde\Gamma_{11}(t-\tau)}\,\chi^\dagger_{11}(t)$$

$$= \frac{1}{\beta}\chi_{11}(t)\,\underbrace{\mathcal{L}^{-1}[\tilde\Gamma_{11}(s)\chi^\dagger_{11}(s)]}_{\mathcal{L}^{-1}[\chi_{11}(s)\tilde\Gamma^\dagger_{11}(s)]^\dagger = \mathcal{L}^{-1}[\chi_{11}(s)\tilde\Gamma_{11}(s)]^\dagger} + \frac{1}{\beta}\mathcal{L}^{-1}[\chi_{11}(s)\tilde\Gamma_{11}(s)]\,\chi^\dagger_{11}(t)$$

Consider now

$$\chi_{11}^{-1} = (s^2 1 + \tilde D_{11} + s\tilde\Gamma_{11}) \to \tilde\Gamma_{11} = \frac{1}{s}\left[\chi_{11}^{-1} - (s^2 1_{11} + \tilde D_{11})\right]$$

$$\chi_{11}(s)\tilde\Gamma_{11}(s) = \frac{1}{s}\chi_{11}(\chi_{11}^{-1} - s^2 1 - \tilde D_{11}) = \frac{1}{s} - s\chi_{11} - \frac{1}{s}\chi_{11}\tilde D_{11}$$

$$= \frac{1}{s} - \mathcal{L}^{-1}[\dot\chi_{11}(t)] - \frac{1}{s}\chi_{11}\tilde D_{11},$$

so that $\mathcal{L}^{-1}[\chi_{11}(s)\tilde\Gamma_{11}(s)] = 1 - \dot\chi_{11}(t) - \int_0^t \chi_{11}(\tau)\,d\tau\,\tilde D_{11}$

Therefore,

$$\mathring{A}_{11}(t) = \frac{1}{\beta}\, \chi_{11}(t)\left[1 - \mathring{\chi}_{11}(t) - \int_0^t \chi_{11}(\tau)\,d\tau \cdot \tilde{D}_{11}\right]^{\dagger}$$

$$+ \frac{1}{\beta}\left[1 - \mathring{\chi}_{11}(t) - \int_0^t \chi_{11}(\tau)\,d\tau\, \tilde{D}_{11}\right] \chi_{11}^{\dagger}(t)$$

$$\cancel{= \frac{1}{\beta}\Big[\chi_{11}(t) - \chi_{11}(t)\,\mathring{\chi}_{11}(t) - \chi_{11}(t)\,\tilde{D}_{11}\int_0^t \chi_{11}^{\dagger}(\tau)\,d\tau}$$

$$\cancel{+ \chi_{11}^{\dagger}(t) - \mathring{\chi}_{11}(t)\,\chi_{11}^{\dagger}(t) - \int_0^t \chi_{11}(\tau)\,d\tau\, \tilde{D}_{11}\, \chi_{11}^{\dagger}(t)\Big]}$$

$$= \frac{1}{\beta}\, \chi_{11}(t)\left[-\mathring{\chi}_{11}(t) + \xi_{11}(t)\right]^{\dagger} + \frac{1}{\beta}\left[-\mathring{\chi}_{11}(t) + \xi_{11}(t)\right] \chi_{11}^{\dagger}(t)$$

$$= \frac{1}{\beta}\left[-\chi_{11}(t)\,\mathring{\chi}_{11}^{\dagger}(t) + \chi_{11}(t)\,\xi_{11}^{\dagger}(t) - \mathring{\chi}_{11}(t)\,\chi_{11}^{\dagger}(t) + \xi_{11}(t)\,\chi_{11}^{\dagger}(t)\right]$$

$$= \frac{1}{\beta}\left[-\frac{d}{dt}\left(\chi_{11}(t)\,\chi_{11}^{\dagger}(t)\right) + \mathring{\xi}_{11}(t)\,\tilde{D}_{11}^{-1}\,\xi_{11}^{\dagger}(t) - \xi_{11}(t)\,\tilde{D}_{11}^{-1}\,\mathring{\xi}_{11}^{\dagger}(t)\right]$$

$$= -\frac{1}{\beta}\,\frac{d}{dt}\left[\chi_{11}(t)\,\chi_{11}^{\dagger}(t) + \xi_{11}(t)\,\tilde{D}_{11}^{-1}\,\xi_{11}^{\dagger}(t)\right],$$

so $A_{11}(t) = -\frac{1}{\beta}\left(\chi_{11}(t)\,\chi_{11}^{\dagger}(t) + \xi_{11}(t)\,\tilde{D}_{11}^{-1}\,\xi_{11}^{\dagger}(t)\right) + C$

But $A_{11}(0) = 0$ by definition of $A_{11}(t)$; thus:

$$0 = -\frac{1}{\beta}\Big(\underset{0}{\underset{\shortparallel}{\chi_{11}(0)}}\,\underset{0}{\underset{\shortparallel}{\chi_{11}^{\dagger}(0)}} + \underbrace{\xi_{11}(0)}_{=1}\,\tilde{D}_{11}^{-1}\,\underbrace{\xi_{11}^{\dagger}(0)}_{=1}\Big) + C,$$

so that $C = \frac{1}{\beta}\tilde{D}_{11}^{-1}$, so that

$$\boxed{A_{11}(t) = -\frac{1}{\beta}\left[\chi_{11}(t)\,\chi_{11}^{\dagger}(t) + \xi_{11}(t)\,\tilde{D}_{11}^{-1}\,\xi_{11}^{\dagger}(t)\right] + \frac{1}{\beta}\tilde{D}_{11}^{-1}}$$

At long times

$$\boxed{A_{\parallel}(t) \to \frac{1}{\beta}\tilde{D}_{\parallel}^{-1}}$$

- Next we consider

$$\dot{A}_{\parallel}(t) = \frac{1}{\beta}\chi_{\parallel}(t)\int_0^t d\tau'\,\tilde{\Gamma}_{\parallel}(t-\tau')\,\dot{\chi}^{+}_{\parallel}(\tau') +$$

$$+\frac{1}{\beta}\int_0^t d\tau\,\chi_{\parallel}(\tau)\,\tilde{\Gamma}_{\parallel}(\tau-t)\,\dot{\chi}^{+}_{\parallel}(t)$$

$$= \frac{1}{\beta}\chi_{\parallel}(t)\,\mathcal{L}^{-1}\left[\tilde{\Gamma}_{\parallel}(s)\,\dot{\chi}^{+}_{\parallel}(s)\right] + \frac{1}{\beta}\,\mathcal{L}^{-1}\left[\chi_{\parallel}(s)\tilde{\Gamma}_{\parallel}(s)\right]\dot{\chi}^{+}_{\parallel}(t)$$

Here $\mathcal{L}[\dot{\chi}_{\parallel}(t)] = s\chi_{\parallel}(s) - \chi_{\parallel}(0) = s\chi_{\parallel}(s)$, so that

$$\left[\tilde{\Gamma}_{\parallel}(s)\,\dot{\chi}^{+}_{\parallel}(s)\right] = \left[\dot{\chi}_{\parallel}(s)\,\tilde{\Gamma}_{\parallel}(s)\right]^{+} =$$

$$= s\left[\chi_{\parallel}(s)\tilde{\Gamma}_{\parallel}(s)\right]^{+} =$$

$$= s\left[\frac{1}{s} - s\chi_{\parallel} - \frac{1}{s}\chi_{\parallel}\tilde{D}_{\parallel}\right]^{+} =$$

$$= s\frac{1}{s}\left(1-\chi_{\parallel}(s)\tilde{D}_{\parallel}\right)^{+} - s^2\chi^{+}_{\parallel} = -\left(s^2\chi_{\parallel}-1\right)^{+} - \left(\chi_{\parallel}(s)\tilde{D}_{\parallel}\right)^{+}$$

$$= -\tilde{D}_{\parallel}\chi^{+}_{\parallel}(s) - \left(s^2\chi_{\parallel}-1\right)^{+},$$

$$\mathcal{L}^{-1}\left[\tilde{\Gamma}_{\parallel}(s)\,\dot{\chi}^{+}_{\parallel}(s)\right] = \mathcal{L}^{-1}\left[\dot{\chi}_{\parallel}(s)\,\tilde{\Gamma}_{\parallel}(s)\right]^{+} =$$

$$= \mathcal{L}^{-1}\left[-\tilde{D}_{\parallel}\chi^{+}_{\parallel}(s) - \left(s^2\chi_{\parallel}-1\right)^{+}\right] = -\tilde{D}_{\parallel}\chi^{+}_{\parallel}(t) - \ddot{\chi}^{+}_{\parallel}(t)$$

so that

$$\dot{A}_{\parallel}(t) = -\frac{1}{\beta}\chi_{\parallel}(t)\left[\tilde{D}_{\parallel}\chi^{+}_{\parallel}(t) + \ddot{\chi}^{+}_{\parallel}(t)\right] + \frac{1}{\beta}\left[1 - \dot{\chi}_{\parallel}(t) - \int_0^t \chi_{\parallel}(\tau)\,d\tau\,\tilde{D}_{\parallel}\right]\dot{\chi}^{+}_{\parallel}(t)$$

$$= -\frac{1}{\beta}\Big[\chi_{11}\tilde{\Delta}_{11}\chi_{11}^{\dagger} + \chi_{11}\ddot{\chi}_{11}^{\dagger} - \xi_{11}\dot{\chi}_{11}^{\dagger} + \dot{\chi}_{11}\dot{\chi}_{11}^{\dagger} \Big]$$

Since $\dot{\xi}_{11} = -\chi_{11}\tilde{\Delta}_{11}$, then

$$\hookrightarrow \dot{A}_{12}(t) = -\frac{1}{\beta}\Big[-\dot{\xi}_{11}\chi_{11}^{\dagger} - \xi_{11}\dot{\chi}_{11}^{\dagger} + \chi_{11}\ddot{\chi}_{11}^{\dagger} + \dot{\chi}_{11}\dot{\chi}_{11}^{\dagger} \Big]$$

$$= -\frac{1}{\beta}\frac{d}{dt}\Big[-\xi_{11}\chi_{11}^{\dagger} + \chi_{11}\dot{\chi}_{11}^{\dagger} \Big]$$

and ~~since~~ hence

$$A_{12}(t) = -\frac{1}{\beta}\left(-\xi_{11}(t)\chi_{11}^{\dagger}(t) + \chi_{11}(t)\dot{\chi}_{11}^{\dagger}(t) \right) + C$$

$$A_{12}(0) = 0 \to -\frac{1}{\beta}\Big(-\underbrace{\xi_{11}(0)}_{=0}\underbrace{\chi_{11}^{\dagger}(0)}_{=0} + \underbrace{\chi_{11}(0)}_{=0}\dot{\chi}_{11}^{\dagger}(0) \Big) + C$$

$\hookrightarrow C = 0,$

$$\boxed{A_{12}(t) = \frac{1}{\beta}\left(\xi_{11}(t)\chi_{11}^{\dagger}(t) - \chi_{11}(t)\dot{\chi}_{11}^{\dagger}(t) \right)}$$

and $A_{12}(t) \to 0$ as $t \to \infty$.

- Finally, we consider

$$\dot{A}_{22}(t) = \frac{1}{\beta}\dot{\chi}_{11}(t)\int_0^t d\tau'\, \tilde{\Gamma}_{11}(t-\tau)\dot{\chi}_{11}^{\dagger}(\tau) + \frac{1}{\beta}\int_0^t d\tau\, \dot{\chi}_{11}(\tau)\tilde{\Gamma}_{11}(\tau - t)\dot{\chi}_{11}^{\dagger}(t)$$

$$= \frac{1}{\beta}\dot{\chi}_{11}(t)\mathcal{L}^{-1}\Big[\tilde{\Gamma}_{11}(s)(s\chi_{11}^{\dagger}(s))\Big] + \frac{1}{\beta}\mathcal{L}^{-1}\big[s\chi_{11}(s)\tilde{\Gamma}_{11}(s)\big]\cdot\dot{\chi}_{11}^{\dagger}(t)$$

$$= \frac{1}{\beta}\dot{\chi}_{11}(t)\Big[-\tilde{\Delta}_{11}\chi_{11}^{\dagger}(t) - \ddot{\chi}_{11}^{\dagger}(t)\Big] + \frac{1}{\beta}\Big[-\chi_{11}(t)\tilde{\Delta}_{11} - \ddot{\chi}_{11}(t)\Big]\dot{\chi}_{11}^{\dagger}(t)$$

$$= \frac{1}{\beta}\Big\{ + \dot{\xi}_{11}(t)\chi_{11}^{\dagger}(t) - \dot{\chi}_{11}\ddot{\chi}_{11}^{\dagger} + \xi_{11}(t)\dot{\chi}_{11}^{\dagger}(t) - \ddot{\chi}_{11}(t)\dot{\chi}_{11}^{\dagger}(t) \Big\}$$

$$= \frac{1}{\beta}\frac{d}{dt}\Big[\xi_{11}(t)\chi_{11}^{\dagger}(t) - \dot{\chi}_{11}(t)\dot{\chi}_{11}^{\dagger}(t) \Big],$$ and hence

$$A_{22}(t) = \frac{1}{\beta}\left(\dot{\xi}_{11}(t)\,\chi_{11}^{+}(t) - \dot{\chi}_{11}(t)\,\dot{\chi}_{11}^{+}(t)\right) + C,$$

$$A_{22}(0) = 0 \equiv \frac{1}{\beta}\left(\dot{\xi}_{11}(0)\,\underbrace{\chi_{11}^{+}(0)}_{=0} - \dot{\chi}_{11}(0)\,\dot{\chi}_{11}^{+}(0)\right) + C$$

From initial conditions on the velocity:

$$v_1(0) \equiv \dot{x}_1(0) = \dot{\xi}_{11}(0)\,x_1(0) + \dot{\chi}_{11}(0)\,\dot{x}_1(0)$$

follows: $\boxed{\dot{\xi}_{11}(0) = 0}$ $\boxed{\dot{\chi}_{11}(0) = 1}$

and therefore,

$$A_{22}(0) = 0 = -\frac{1}{\beta} + C \Rightarrow \boxed{C = \frac{1}{\beta}}$$

and

$$\boxed{A_{22}(t) = \frac{1}{\beta}\left[\mathbb{1} + \dot{\xi}_{11}(t)\,\chi_{11}^{+}(t) - \dot{\chi}_{11}(t)\,\dot{\chi}_{11}^{+}(t)\right]}$$

$$\boxed{A_{22}(t) \to \frac{1}{\beta}\mathbb{1} \text{ at } t \to \infty}$$

5. Therefore, $y_1(t)$ and $y_2(t)$ are Gaussian with the distribution

~~$\mathcal{P}(y_1, y_2) \sim \exp[$~~

$$\mathcal{P}(y_1, y_2) \sim \exp\left[-\frac{1}{2}y_1^{+} A^{-1} y_2\right],$$

~~where~~ At long times

$$A^{-1} \to \begin{pmatrix} \frac{1}{\beta} D_{11}^{-1} & 0 \\ 0 & \frac{1}{\beta}\mathbb{1} \end{pmatrix}$$

and $\boxed{A^{-1}(t) \to \begin{pmatrix} \beta \tilde{D}_{11} & 0 \\ 0 & \beta \mathbb{1}_{11} \end{pmatrix}}$ for $t \to \infty$

Also, $y_1(t) \to X_1(\infty)$, $y_2(t) \to \dot{X}_1(\infty)$ at long times.

So,

$$\mathcal{P}(X_1(\infty), \dot{X}_1(\infty)) \sim \exp\left[-\frac{\beta}{2} X_1^\dagger(\infty)\, \tilde{D}_{11} X_1(\infty) - \frac{\beta}{2} \dot{X}_1^\dagger(\infty) \dot{X}_1(\infty) \right]$$

$$\sim \exp\left[-\frac{\beta}{2} \left(X_1^\dagger(\infty) \tilde{D}_{11} X_1(\infty) + \dot{X}_1^\dagger(\infty) \dot{X}_1(\infty) \right) \right]$$

Consequently, since the actual displacements and velocities are related to X_1, $\dot{X}_1$ as:

$$X_1(t) = \sqrt{M_{11}}\, u_1(t), \quad \dot{X}_1(t) = \sqrt{M_{11}}\, \dot{u}_1(t)$$

we obtain

$$\boxed{\mathcal{P}(u_1, \dot{u}_1) \sim \exp\left[-\beta\, \mathcal{H}_1 \right],}$$

$$\mathcal{H}_1 = \frac{1}{2} u_1^\dagger \left(\sqrt{M_{11}}\, \tilde{D}_{11} \sqrt{M_{11}} \right) u_1 + \frac{1}{2} \dot{u}_1^\dagger \sqrt{M_{11}} \sqrt{M_{11}}\, \dot{u}_1$$

$$\boxed{\mathcal{H}_1 = \frac{1}{2} u_1^\dagger \tilde{\Phi}_{11} u_1 + \frac{1}{2} \dot{u}_1^\dagger M_{11} \dot{u}_1}$$

which is the Hamiltonian of ~~the~~ region 1 with effective interaction:

$$\tilde{\Phi}_{11} = M_{11}^{+1/2} \tilde{D}_{11} M_{11}^{+1/2} = M_{11}^{1/2} \left(D_{11} - D_{12} D_{22}^{-1} D_{21} \right) M_{11}^{+1/2}$$

$$= \Phi_{11} - \Phi_{12} \Phi_{22}^{-1} \Phi_{21}$$

This corresponds to the total Hamiltonian in which atoms in region 2 are in instantaneous equilibrium with atoms in 1 clamped in positions u_1.