Solution of Kac-Zwanzig

6. $H = H_p + H_{bath} =$

$$= P^2/2M + U(X) + \sum \tfrac{1}{2} p_i^2 + \sum \tfrac{1}{2}\omega_j^2 (q_j - \gamma_j X/\omega_j^2)^2$$

$$\frac{\partial H}{\partial p_i} = \dot{q}_i \quad , \quad \frac{\partial H}{\partial q_i} = -\dot{p}_i$$

(1) $$\frac{dX}{dt} = \frac{\partial H}{\partial P} = \frac{P}{M}$$

(*) $$\frac{dP}{dt} = -U'(X) + \sum \gamma_j (q_j - \gamma_j X/\omega_j^2) =$$

$$= -U'(X) + \sum \gamma_j q_j - \sum \left(\frac{\gamma_j}{\omega_j}\right)^2 X(t)$$

$$\dot{q}_i = p_i$$

$$\dot{p}_i = -\omega_j^2 (q_j - \gamma_j X/\omega_j^2)$$

(2) $$\ddot{q}_j(t) = -\omega_j^2 q_j(t) + \gamma_j X(t)$$

~~Fourier transform~~

~~$-k^2 q_j(k) + \omega_j^2 q_j(k) = \gamma_j X(k)$~~

~~$q_j(k) = \frac{\gamma_j}{\omega_j^2 - k^2} X(k)$~~

It's no good to solve with F.T because of the initial conditions. We must use the initial conditions for the Fluctuation-Dissipation.

So we Perform a L.T

Initial conditions

$q(0) = q_0$

$\dot{q}(0) = p_0$

$$q(s) = \int_0^\infty e^{-st} q(t)\, dt$$

$$\int_0^\infty e^{-st} \ddot{q}(t) dt = e^{-st} \dot{q}(t) \Big|_0^\infty + s \int_0^\infty e^{-st} \dot{q}(t)\, dt =$$

$$= -p(0) + s e^{-st} q(t) \Big|_0^\infty + s^2 \int_0^\infty e^{-st} q(t)\, dt$$

$$= -p(0) - s q(0) + s^2 q(s)$$

$$q_j(s) = \frac{\gamma_j X(s)}{s^2 + \omega_j^2} + \frac{p(0) + s q(0)}{\omega^2 + s^2}$$

Convolution

$$\frac{1}{s^2 + \omega_j^2} \underset{L.T}{\Longleftrightarrow} = \frac{\sin(\omega_j t)}{\omega_j}$$

$$\frac{s}{\omega_j^2 + s^2} \underset{L.T}{\Longleftrightarrow} = \cos(\omega_j t)$$

$$q_j(t) = \frac{\gamma_j}{\omega_j} \int_0^t x(t-t') \sin(\omega_j t')\, dt' + \frac{p_j(0)}{\omega_j} \sin(\omega_j t) + q_j(0) \cos(\omega_j t)$$

$$= -\frac{\gamma_j}{\omega_j^2} x(t-t') \cos(\omega_j t') \Big|_0^t - \int_0^t \frac{dx(t-t')}{dt'} \frac{\gamma_j}{\omega_j^2} \cos(\omega_j t')\, dt'$$

Integration by parts

the minus sign is from $(t-t')$

$$+ \frac{p_j(0)}{\omega_j} \sin(\omega_j t) + q_j(0) \cos(\omega_j t)$$

$$q_j(t) - \frac{\gamma_i}{\omega_j^2} X(t) = -\int_0^t \frac{P(t-t')}{M}\left(\frac{\gamma_j}{\omega_j^2}\right)\cos(\omega_j t')\,dt'$$

$$-X(0)\left(\frac{\gamma_i}{\omega_j^2}\right)\cos(\omega_j t) + \frac{P_j(0)}{\omega_j}\sin(\omega_j t) + q_j(0)\cos(\omega_j t)$$

and from (*) we get

$$\frac{dP}{dt} = -U(X') - \int_0^t \frac{P(t-t')}{M}\sum\left(\frac{\gamma_i}{\omega_j}\right)^2\cos(\omega_j t')\,dt'$$

~~$-X_0\sum\left(\frac{\gamma_i}{\omega_j}\right)^2\cos(\omega_j t) + P_i$~~

$$+\sum P_j(0)\left(\frac{\gamma_j}{\omega_j}\right)\sin(\omega_j t) + \sum \gamma_j\left(q_j(0) - \frac{\gamma_i}{\omega_j^2}X(0)\right)\cos(\omega_j t)$$

$$\frac{dP}{dt} = -U(x') - \int_0^t dt'\,\eta(t')\frac{P(t-t')}{M}\,dt' + F(t)$$

$$\eta(t) = \sum_j\left(\frac{\gamma_i}{\omega_j}\right)^2\cos(\omega_j t)$$

$$F(t) = \sum_j P_j(0)\left(\frac{\gamma_i}{\omega_j}\right)\sin(\omega_j t) + \sum_j \gamma_j\left(q_j(0) - \frac{\gamma_i}{\omega_j^2}X(0)\right)\cdot\cos(\omega_j t)$$

At $t=0$, the bath particles are assumed to be in thermal equilibrium and we suppous that $X(0)$ is known

$$\text{Prob}(q(0)\,p(0)\mid X(0)\text{ is known}) \propto \exp\left[-H_{bath}/kT\right]$$

$$H_{bath} = \Sigma \frac{1}{2} p_j^2 + \Sigma \frac{1}{2}\omega_j^2 (q_j - \gamma_j X(0)/\omega_j^2)^2$$

It is a gaussian distribution so we get

$$\langle p_j^2(0)\rangle = k_b T \qquad \langle p_j \rangle = 0$$

$$\left\langle \left(q_j(0) - \frac{\gamma_j X(0)}{\omega_j^2}\right)^2\right\rangle = \frac{k_b T}{\omega_j^2} \qquad \left\langle q_j(0) - \frac{\gamma_j X(0)}{\omega_j^2}\right\rangle = 0$$

Our force is a linear combination of p_j and $\left(q_j(0) - \frac{\gamma_j X(0)}{\omega_j^2}\right)$

$$\langle F(t)\rangle = 0$$

$$\langle F(t) F(t')\rangle = \sum_{jk} \langle p_j p_k\rangle \left(\frac{\gamma_j}{\omega_j}\right)\left(\frac{\gamma_k}{\omega_k}\right) \sin(\omega_j t)\sin(\omega_k t')$$

$$+ \sum_{jk} \gamma_j \gamma_k \left\langle \left(q_j - \frac{\gamma_j}{\omega_j^2} X(0)\right)\left(q_k - \frac{\gamma_k}{\omega_k^2} X(0)\right)\right\rangle \cos(\omega_j t)\cos(\omega_k t')$$

$$+ \sum_{jk} \left\langle p_j \left(q_k - \frac{\gamma_k}{\omega_k^2} X(0)\right)\right\rangle \cdot [\ \ ]$$

$$\langle p_j p_k \rangle = \delta_{jk} k_b T$$

$$\left\langle \left(q_j - \frac{\gamma_j}{\omega_j^2} X(0)\right)\left(q_k - \frac{\gamma_k}{\omega_k^2} X(0)\right)\right\rangle = \delta_{jk} \frac{k_b T}{\omega_j^2}$$

$$\left\langle p_j \left(q_j - \frac{\gamma_j}{\omega_j^2} X(0)\right)\right\rangle = 0$$

$$\langle F(t) F(t')\rangle = k_b T \sum_j \left[\left(\frac{\gamma_j}{\omega_j}\right)^2 \sin(\omega_j t)\sin(\omega_j t') + \left(\frac{\gamma_j}{\omega_j}\right)^2 \cos(\omega_j t)\cos(\omega_j t')\right]$$

$$\sin(\omega_j t)\sin(\omega_j t') = \frac{1}{2}\left[\cos(\omega_j(t-t')) - \cos(\omega_j(t+t'))\right]$$
$$+ \cos(\omega_j t)\cos(\omega_j t') = \frac{1}{2}\left[\cos(\omega_j(t-t')) + \cos(\omega_j(t+t'))\right]$$

$$\overline{\qquad\qquad \cos(\omega_j(t-t')) \qquad}$$

$$\boxed{\begin{aligned} \langle F(t)F(t')\rangle &= k_B T \sum_j \left(\frac{\gamma_j}{\omega_j}\right)^2 \cos(\omega_j(t-t')) \\ &= k_B T\, \eta(t-t') \end{aligned}}$$

White noise: treat frequency distribution as continuos with distribution

$$g(\omega) = \begin{cases} 3\omega^2/\omega_d^2 & \omega < \omega_d \\ 0 & \omega > \omega_d \end{cases}$$

the sum goes to $N\int d\omega\, g(\omega)$

and suppose the coupling constants are all the same $\gamma / N^{1/2}$

$$\eta(t) = \sum\left(\frac{\gamma_i}{\omega_i}\right)^2 \cos(\omega_i t) = N\int_0^{\omega_d} \frac{\gamma^2}{N\omega^2}\cdot\frac{3\omega^2}{\omega_d^2}\cos(\omega t)\,d\omega$$

$$= \frac{3\gamma^2}{\omega_d^2}\int_0^{\omega_d}\cos(\omega t)\,d\omega = \frac{3\gamma^2}{\omega_d^2}\,\frac{\sin(\omega_d t)}{t}$$

using a relation ~~sin~~ $\lim_{\alpha\to\infty} \frac{\sin\alpha x}{\pi x} = \delta(x)$ and supposing that $P(t)$ is varing slowly over times of the order $\frac{1}{\omega_d}$ we can replace the $\frac{\sin\omega_d t}{t}$ by $\pi\delta(t)$

we get $\eta(t) = \frac{3\gamma^2\pi}{\omega_d^2}$

and $\langle F(t) F(t') \rangle = \frac{k_B T \cdot 3\pi\gamma^2}{\omega_d^2} \delta(t-t')$