3.13. Particle in Heat Bath

Consider a particle of mass M subject to a potential $V(x)$ while moving in a dissipative medium at a constant temperature. Such medium is usually called a heat bath.

We can simulate a heat bath as a collection of a huge number of harmonic oscillators $X_i(\tau)$; $i = 1, 2, 3, \ldots$ of various masses M_i & frequencies Ω_i.

The imaginary-time evolution amplitude of the particle is therefore

$$(x_b\ \beta\hbar \mid x_a\ 0) = \left(\prod_i \oint \mathcal{D} X_i(\tau)\right) \int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}\, x(\tau) \left(\prod_i \frac{e^{-\mathcal{A}_i[c_i]/\hbar}}{Z_i}\right) e^{-\mathcal{A}/\hbar} \qquad (3.396)$$

where

$$\mathcal{A}_i[c_i] = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} M_i \left(\dot{X}_i^2 + \Omega_i^2 X_i^2\right) - c_i X_i x\right] \qquad (3.396a)$$

$$\mathcal{A} = \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} M \dot{x}^2 + V(x)\right] \qquad (3.396b)$$

$$Z_i = \oint \mathcal{D} X_i(\tau)\, e^{-\mathcal{A}_i[0]/\hbar} = \frac{1}{2\sinh\left(\frac{1}{2}\beta\hbar\Omega_i\right)} \qquad (3.397)$$

Using (3.305-6) with $j = c_i x$, we have

$$Z_i[c_i] = \oint \mathcal{D} X_i(\tau)\, e^{-\mathcal{A}_i[c_i]/\hbar}$$

$$= Z_i \exp\left\{\frac{c_i^2}{2 M_i \hbar} \int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, x(\tau)\, G^p_{\Omega_i^2, e}(\tau - \tau')\, x(\tau')\right\} \qquad (3.398a)$$

(3.396) thus becomes

$$(x_b\ \beta\hbar \mid x_a\ 0) = \int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}\, x(\tau) \left(\prod_i \frac{Z_i[c_i]}{Z_i}\right) e^{-\mathcal{A}/\hbar}$$

$$= \int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}\, x(\tau)\ e^{-\mathcal{A}_{\text{bath}}/\hbar}\, e^{-\mathcal{A}/\hbar} \qquad (3.398)$$

where

$$\mathcal{A}_{\text{bath}} = -\sum_i \frac{c_i^2}{2 M_i} \int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, x(\tau)\, G^p_{\Omega_i^2, e}(\tau - \tau')\, x(\tau')$$

$$= -\frac{1}{2} \int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, x(\tau)\, \alpha(\tau - \tau')\, x(\tau') \qquad (3.399)$$

and

$$\alpha(\tau - \tau') = \sum_i \frac{c_i^2}{M_i} G^p_{\Omega_i^2, e}(\tau - \tau') \qquad (3.400a)$$

is the weighted periodic correlation function.

Using (3.248), we have

$$\alpha(\tau - \tau') = \sum_i \frac{c_i^2}{M_i} \frac{1}{2\Omega_i} \frac{\cosh \Omega_i \left(\frac{1}{2}\beta\hbar - |\tau - \tau'|\right)}{\sinh\left(\frac{1}{2}\beta\hbar\Omega_i\right)} \qquad (3.400)$$

Owing to the periodicity of $G^p_{\Omega_i^2, e}(\tau - \tau')$, we can expand $\alpha(\tau - \tau')$ as a Fourier series

$$\alpha(\tau - \tau') = \frac{1}{\beta\hbar} \sum_{m=-\infty}^{\infty} \alpha_m\, e^{-i\omega_m(\tau - \tau')} \qquad \omega_m = \frac{2\pi}{\beta\hbar} m \qquad (3.401)$$

where

$$\alpha_m = \int_0^{\beta\hbar} d\,\tau\,\alpha(\tau)\,e^{i\,\omega_m\,\tau}$$

$$= \sum_i \frac{c_i^2}{M_i} \frac{1}{2\,\Omega_i \sinh\left(\frac{1}{2}\,\beta\,\hbar\,\Omega_i\right)} \int_0^{\beta\hbar} d\,\tau\,e^{i\,\omega_m\,\tau} \cosh\Omega_i\left(\frac{1}{2}\,\beta\,\hbar - \tau\right)$$

Using

$$\int_0^{\beta\hbar} d\,\tau\,e^{i\,\omega_m\,\tau} \cosh\Omega_i\left(\frac{1}{2}\,\beta\,\hbar - \tau\right)$$

$$= \frac{1}{2} \int_0^{\beta\hbar} d\,\tau\,e^{i\,\omega_m\,\tau}\left(e^{\Omega_i\left(\frac{1}{2}\beta\,\hbar - \tau\right)} + e^{-\Omega_i\left(\frac{1}{2}\beta\,\hbar - \tau\right)}\right)$$

$$= \frac{1}{2}\left[\frac{e^{\beta\,\hbar\,\Omega_i/2}}{i\,\omega_m - \Omega_i}\left(e^{-\beta\,\hbar\,\Omega_i} - 1\right) + \frac{e^{-\beta\,\hbar\,\Omega_i/2}}{i\,\omega_m + \Omega_i}\left(e^{\beta\,\hbar\,\Omega_i} - 1\right)\right] \qquad \left[\ \omega_m = \frac{2\,\pi}{\beta\,\hbar}\,m\ \right]$$

$$= \frac{1}{2}\left(\frac{1}{i\,\omega_m - \Omega_i} - \frac{1}{i\,\omega_m + \Omega_i}\right)\left(e^{-\beta\,\hbar\,\Omega_i/2} - e^{\beta\,\hbar\,\Omega_i/2}\right)$$

$$= \frac{1}{2}\left(\frac{2\,\Omega_i}{-\omega_m^2 - \Omega_i^2}\right)\left(e^{-\beta\,\hbar\,\Omega_i/2} - e^{\beta\,\hbar\,\Omega_i/2}\right)$$

$$= \frac{2\,\Omega_i}{\omega_m^2 + \Omega_i^2} \sinh\beta\,\hbar\,\Omega_i$$

we have

$$\alpha_m = \sum_i \frac{c_i^2}{M_i} \frac{1}{\omega_m^2 + \Omega_i^2} \tag{3.402}$$

Alternatively, we can use

$$G^p_{\omega^2,e}(\tau,\ \tau') = \frac{1}{2\,\omega} \sum_{n=-\infty}^{\infty} e^{-\omega\,|\,\tau - \tau' + n\,\beta\,\hbar\,|} \tag{3.277}$$

to write (3.399) as

$$\mathcal{A}_{\text{bath}} = -\sum_i \frac{c_i^2}{2\,M_i} \int_0^{\beta\,\hbar} d\,\tau \frac{1}{2\,\Omega_i} \sum_{n=-\infty}^{\infty} \int_0^{\beta\,\hbar} d\,\tau'\,x(\tau)\,e^{-\Omega_i\,|\,\tau - \tau' + n\,\beta\,\hbar\,|}\,x(\tau')$$

$$= -\sum_i \frac{c_i^2}{2\,M_i} \int_0^{\beta\,\hbar} d\,\tau \frac{1}{2\,\Omega_i} \int_{-\infty}^{\infty} d\,\tau'\,x(\tau)\,e^{-\Omega_i\,|\,\tau - \tau'\,|}\,x(\tau')$$

$$= -\frac{1}{2} \int_0^{\beta\,\hbar} d\,\tau \int_{-\infty}^{\infty} d\,\tau'\,x(\tau)\,\alpha_0(\tau - \tau')\,x(\tau') \tag{3.403}$$

where

$$\alpha_0(\tau - \tau') = \sum_i \frac{c_i^2}{2\,M_i\,\Omega_i}\,e^{-\Omega_i\,|\,\tau - \tau'\,|} \tag{3.404}$$

This can be put into an integral form by defining the spectral density of the bath as

$$\rho_b(\omega) = 2\,\pi \sum_i \frac{c_i^2}{2\,M_i\,\Omega_i}\,\delta(\omega - \Omega_i) \tag{3.405}$$

so that, since $\Omega_i \geq 0$,

$$\sum_i \frac{c_i^2}{2\,M_i\,\Omega_i} f(\Omega_i) = \sum_i \frac{c_i^2}{2\,M_i\,\Omega_i} \int_0^{\infty} d\,\omega\,\delta(\omega - \Omega_i)\,f(\omega)$$

$$= \int_0^{\infty} \frac{d\,\omega}{2\,\pi}\,\rho_b(\omega)\,f(\omega) \tag{3.405a}$$

(3.404) thus becomes

$$\alpha_0(\tau-\tau') = \int_0^\infty \frac{d\,\omega}{2\,\pi}\,\rho_b(\omega)\,e^{-\omega|\tau-\tau'|} \tag{3.406}$$

Similarly, (3.400) & (3.402) become

$$\alpha(\tau-\tau') = \int_0^\infty \frac{d\,\omega}{2\,\pi}\,\rho_b\,(\omega)\,\frac{\cosh\omega\left(\frac{1}{2}\,\beta\,\hbar - \left|\,\tau-\tau'\,\right|\,\right)}{\sinh\left(\frac{1}{2}\,\beta\,\hbar\,\omega\right)} \tag{3.407}$$

$$\alpha_m = \int_0^\infty \frac{d\,\omega}{2\,\pi}\,\rho_b\,(\omega)\,\frac{2\,\omega}{\omega_m^2 + \omega^2} \tag{3.408}$$

Setting $m = 0$ in (3.402) & (3.408) gives

$$\alpha_0 = \sum_i \frac{c_i^2}{M_i}\,\frac{1}{\Omega_i^2} = \int_0^\infty \frac{d\,\omega}{2\,\pi}\,\rho_b(\omega)\,\frac{2}{\omega} \tag{3.408a}$$

Using

$$\frac{2\,\omega}{\omega_m^2 + \omega^2} = \frac{2}{\omega}\left(1 - \frac{\omega_m^2}{\omega_m^2 + \omega^2}\right)$$

we can write (3.408) as

$$\alpha_m = \int_0^\infty \frac{d\,\omega}{2\,\pi}\,\rho_b(\omega)\left[\,\frac{2}{\omega} - \frac{2\,\omega_m^2}{\omega\left(\omega_m^2 + \omega^2\right)}\,\right]$$

$$= \alpha_0 - g_m \tag{3.409}$$

where

$$g_m = \int_0^\infty \frac{d\,\omega}{2\,\pi}\,\rho_b(\omega)\,\frac{2\,\omega_m^2}{\omega\left(\omega_m^2 + \omega^2\right)} \tag{3.413}$$

$$= \sum_i \frac{c_i^2}{2\,M_i\,\Omega_i}\,\frac{2\,\omega_m^2}{\Omega_i\left(\omega_m^2 + \Omega_i^2\right)} \quad \text{[(3.405a) used.]} \tag{3.413a}$$

Using (3.409), we write (3.401) as

$$\alpha(\tau-\tau') = \frac{1}{\beta\,\hbar}\sum_{m=-\infty}^{\infty}(\alpha_0 - g_m)\,e^{-i\,\omega_m(\tau-\tau')}$$

$$= \alpha_0\,\delta^P(\tau-\tau') - g(\tau-\tau') \tag{3.410}$$

where

$$\delta^P(\tau-\tau') = \frac{1}{\beta\,\hbar}\sum_{m=-\infty}^{\infty} e^{-i\,\omega_m(\tau-\tau')}$$

$$= \sum_{n=-\infty}^{\infty}\delta(\tau-\tau'-n\,\beta\,\hbar) \quad \text{[(1.197) used.]} \tag{3.411}$$

is the periodic δ-function [see (3.279)] and

$$g(\tau-\tau') = \frac{1}{\beta\,\hbar}\sum_{m=-\infty}^{\infty} g_m\,e^{-i\,\omega_m(\tau-\tau')} \tag{3.412}$$

is the subtracted correlation function.

Using (3.410), we decompose the bath action (3.399) as

$$\mathcal{A}_{\text{bath}}[x] = -\frac{1}{2}\int_0^{\beta\hbar} d\,\tau\int_0^{\beta\hbar} d\,\tau'\,x(\tau)\left[\,\alpha_0\,\delta^P(\tau-\tau') - g(\tau-\tau')\,\right]x(\tau')$$

$$= \mathcal{A}_{\text{loc}} + \mathcal{A}'_{\text{bath}}[x] \tag{3.414}$$

where

$$\mathcal{A}'_{\text{bath}}[x] = \frac{1}{2}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, x(\tau)\, g(\tau-\tau')\, x(\tau') \qquad (3.415)$$

and

$$\begin{aligned}\mathcal{A}_{\text{loc}} &= -\frac{1}{2}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, x(\tau)\, \alpha_0\, \delta^P(\tau-\tau')\, x(\tau') \\ &= -\frac{1}{2}\alpha_0 \int_0^{\beta\hbar} d\tau\, x^2(\tau) \end{aligned} \qquad (3.416)$$

is a local action corresponding to an effective harmonic potential

$$V_b = -\frac{1}{2}\alpha_0\, x^2 \equiv \frac{1}{2} M\,\Delta\omega^2\, x^2 \qquad (3.417a)$$

where the frequency shift $\Delta\omega^2$ is defined as

$$\begin{aligned} M\,\Delta\omega^2 &\equiv -\alpha_0 \\ &= -\int_0^{\infty}\frac{d\omega}{2\pi}\rho_b(\omega)\,\frac{2}{\omega} \qquad [\,(3.408a)\text{ used.}] \\ &= -\sum_i \frac{c_i^2}{M_i}\frac{1}{\Omega_i^2} \end{aligned} \qquad (3.417)$$

(3.416) thus becomes

$$\begin{aligned}\mathcal{A}_{\text{loc}} &= \int_0^{\beta\hbar} d\tau\, V_b \\ &= \frac{1}{2} M\,\Delta\omega^2 \int_0^{\beta\hbar} d\tau\, x^2(\tau) \end{aligned} \qquad (3.418)$$

V_b can be combined with V to give a renormalized potential

$$V_{\text{ren}}(x) = V(x) + V_b(x) \;= V(x) + \frac{1}{2} M\,\Delta\omega^2\, x^2 \qquad (3.419)$$

so that the evolution amplitude (3.398) becomes

$$(\,x_b\;\beta\hbar\;|\;x_a\,0\,) = \int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}\,x(\tau)\; e^{-\mathcal{A}'_{\text{bath}}/\hbar}\, e^{-\mathcal{A}_{\text{ren}}/\hbar} \qquad (3.420)$$

where

$$\begin{aligned}\mathcal{A}_{\text{ren}} &= \mathcal{A} + \mathcal{A}_{\text{loc}} \\ &= \int_0^{\beta\hbar} d\tau \left[\frac{1}{2} M\,\dot{x}^2 + V_{\text{ren}}(x)\right] \end{aligned} \qquad (3.420a)$$

(3.412) gives

$$\begin{aligned}\int_0^{\beta\hbar} d\tau\, g(\tau-\tau') &= \frac{1}{\beta\hbar}\sum_{m=-\infty}^{\infty} g_m\, e^{i\omega_m\tau'} \int_0^{\beta\hbar} d\tau\, e^{-i\omega_m\tau} \\ &= \frac{1}{\beta\hbar}\sum_{m=-\infty}^{\infty} g_m\, \frac{e^{i\omega_m\tau'}}{-i\,\omega_m}\left(e^{-i\,\omega_m\beta\hbar} - 1\right) \qquad \left[\,\omega_m = \frac{2\pi}{\beta\hbar}m\,\right] \\ &= 0 \\ &= \int_0^{\beta\hbar} d\tau'\, g(\tau-\tau') \end{aligned} \qquad (3.421)$$

Together with

$$x(\tau)\,x(\tau') = \frac{1}{2}\left\{x^2(\tau) + x^2(\tau') - [\,x(\tau) - x(\tau')\,]^2\right\} \qquad (3.422)$$

(3.415) becomes

$$\mathcal{A}'_{\text{bath}}[x] = \frac{1}{2}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau'\, g(\tau-\tau')\,\frac{1}{2}\left\{x^2(\tau) + x^2(\tau') - \left[\,x(\tau) - x(\tau')\,\right]^2\right\}$$

$$= -\frac{1}{4} \int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau' g(\tau - \tau') \left[x(\tau) - x(\tau')\right]^2 \qquad (3.423)$$

If Ω_i is densely distributed, $\rho_b(\omega)$ is continuous. As will be shown in (18.208) & (18.317), an oscillator heat bath introduces a friction force F_v into the classical eq. of motion. For the usual form

$$F_v = -M\gamma\dot{x}$$

(18.208) & (18.317) give

$$\rho_b(\omega) \approx 2M\gamma\omega \qquad (3.424)$$

which is characteristic of Ohmic dissipation.

Typical frictional forces usually vanish at high ω. This can be approximated by replacing (3.424) with the Drude form

$$\rho_b(\omega) \approx 2M\gamma\omega \frac{\omega_D^2}{\omega_D^2 + \omega^2} \qquad (3.425)$$

where $\frac{2\pi}{\omega_D} = \tau_D$ is the Drude's relaxation time.

For short times $\tau << \tau_D$, high frequencies $\omega = \frac{2\pi}{\tau} >> \omega_D$ dominates.

$$\rightarrow \qquad \rho_b(\omega) \approx 2M\gamma \frac{1}{\omega} \approx 0$$

and there is no dissipation.

For large ω_D,

$$\rho_b(\omega) \approx 2M\gamma\omega\left(1 - \frac{\omega^2}{\omega_D^2}\right)$$

approaches the Ohmic dissipation.

Inserting (3.425) into (3.413), we have

$$g_m = 4M\gamma\omega_D^2\omega_m^2 \int_0^\infty \frac{d\omega}{2\pi} \frac{1}{(\omega_D^2 + \omega^2)(\omega_m^2 + \omega^2)}$$

$$= 2M\gamma\omega_D^2\omega_m^2 \int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{1}{(\omega_D^2 + \omega^2)(\omega_m^2 + \omega^2)}$$

$$= 2M\gamma\omega_D^2\omega_m^2 i \sum_j \text{Res}\left[\frac{1}{(\omega_D^2 + \omega^2)(\omega_m^2 + \omega^2)};\ \omega_j\right]$$

Closing the contour in the upper plane, we have $\omega_j = i\omega_D,\ i\,|\,\omega_m\,|$.

$$\rightarrow \qquad g_m = 2M\gamma\omega_D^2\omega_m^2 i\left[\frac{1}{2i\omega_D(\omega_m^2 - \omega_D^2)} + \frac{1}{2i\,|\,\omega_m\,|\,(\omega_D^2 - \omega_m^2)}\right]$$

$$= M\gamma\omega_D\,|\,\omega_m\,|\,\frac{|\,\omega_m\,| - \omega_D}{\omega_m^2 - \omega_D^2}$$

$$= M\gamma\frac{\omega_D\,|\,\omega_m\,|}{|\,\omega_m\,| + \omega_D} \qquad (3.426)$$

Note: Closing the contour in the lower plane gives $\omega_j = -i\omega_D,\ -i\,|\,\omega_m\,|$. Together with an overall negative sign due to the clockwise sense of the contour, (3.426) is again obtained.

Setting

$$g_m \equiv M\,|\,\omega_m\,|\,\gamma_m \qquad (3.427)$$

$$\rightarrow \qquad \gamma_m = \gamma \; \frac{\omega_D}{|\,\omega_m\,| + \omega_D} \tag{3.428}$$

Result for the Ohmic dissipation can be obtained by setting $\omega_D \to \infty$. (3.428) thus becomes

$$\gamma_m \to \gamma \tag{3.428a}$$

The Drude form spectral density (3.425) gives rise to a frequency shift [see (3.417)]

$$\begin{aligned}
\Delta\omega^2 &= -\frac{1}{M} \int_0^\infty \frac{d\,\omega}{2\,\pi}\, \rho_b(\omega)\, \frac{2}{\omega} \\
&= -4\,\gamma\,\omega_D^2 \int_0^\infty \frac{d\,\omega}{2\,\pi}\, \frac{1}{\omega_D^2 + \omega^2} \\
&= -2\,\gamma\,\omega_D^2\, i\, \mathrm{Res}\left[\frac{1}{\omega_D^2 + \omega^2};\; i\,\omega_D\right] \\
&= -2\,\gamma\,\omega_D^2\, i\, \frac{1}{2\,i\,\omega_D} \\
&= -\gamma\,\omega_D
\end{aligned} \tag{3.429}$$

which goes to $-\infty$ for Ohmic dissipation $\omega_D \to \infty$.