Models for quantum dissipation

Instead of trying alternatives for the canonical quantization procedure to dissipative systems we shall appeal to the system – plus – reservoir approach . Once the behavior of the complete system is known one traces out the environment degrees of freedom in order to describe the effective dynamical or equilibrium properties of the system of interest.

We propose a model of the system coupled to a bath of non-interacting harmonic oscillators with a given spectral function in such a way that Brownian motion is recovered in the classical limit.

The minimal model

We assume the coupled system can be described by

Total lagrangean
$$L = L_S + L_I + L_R + L_{CT}$$

Lagrangean of the system
$$L_S = \frac{1}{2}\, M\, \dot{q}^2 - V(q)$$

Interaction lagrangean
$$L_I = \sum_k C_k\, q_k\, q,$$

Lagrangean of the reservoir
$$L_R = \sum_k \frac{1}{2}\, m_k\, \dot{q}_k^2 - \sum_k \frac{1}{2}\, m_k\, \omega_k^2\, q_k^2$$

Counter-term
$$L_{CT} = -\sum_k \frac{1}{2}\, \frac{C_k^2}{m_k\, \omega_k^2}\, q^2$$

Equations of motion

$$M\ddot{q} = -V'(q) + \sum_k C_k\, q_k - \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\, q$$

$$m_k\, \ddot{q}_k = -m_k\, \omega_k^2\, q_k + C_k\, q$$

Laplace transform of the kth coordinate of the bath

$$\tilde{q}_k(s) = \frac{\dot{q}_k(0)}{s^2 + \omega_k^2} + \frac{s\, q_k(0)}{s^2 + \omega_k^2} + \frac{C_k\, \tilde{q}(s)}{m_k\ (s^2 + \omega_k^2)}$$

Equation of motion of the variable of interest as a function of time

$$M\ddot{q} + V'(q) + \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\, q \;=\; \frac{-1}{2\,\pi\, i}\int_{\varepsilon - i\,\infty}^{\varepsilon + i\,\infty} \sum_k C_k \left\{ \frac{\dot{q}_k(0)}{s^2 + \omega_k^2} + \frac{s\, q_k(0)}{s^2 + \omega_k^2} \right\} e^{s\,t}\, ds$$

$$+ \sum_k \frac{C_k^2}{m_k} \frac{1}{2\,\pi\, i} \int_{\varepsilon - i\,\infty}^{\varepsilon + i\,\infty} \frac{\tilde{q}(s)}{s^2 + \omega_k^2}\, e^{s\,t}\, ds.$$

One rewrites

$$M\ddot{q} + V'(q) + \sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\frac{1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty}\frac{s^2\,\tilde{q}(s)}{s^2+\omega_k^2}\,e^{s\,t}\,ds$$

$$= -\frac{1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty}\sum_k C_k\left\{\frac{\dot{q}_k(0)}{s^2+\omega_k^2}+\frac{s\,q_k(0)}{s^2+\omega_k^2}\right\}e^{s\,t}\,ds,$$

The last term on the LHS is

$$\frac{d}{dt}\left\{\sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\frac{1}{2\,\pi\,i}\int_{\varepsilon-i\,\infty}^{\varepsilon+i\,\infty}\frac{s\,\tilde{q}(s)}{s^2+\omega_k^2}\,e^{s\,t}\,ds\right\}$$

or $$\frac{d}{dt}\left\{\sum_k \frac{C_k^2}{m_k\,\omega_k^2}\int_0^t \cos\left[\omega_k\,\left(t-t'\right)\right]\,q(t')\,dt'\right\}.$$

Defining the spectral function $J(\omega) = \frac{\pi}{2} \sum_k \frac{C_k^2}{m_k\, \omega_k}\, \delta\left(\omega - \omega_k\right),$

one gets $$\sum_k \frac{C_k^2}{m_k\, \omega_k^2} \cos\left[\omega_k\ (t - t')\right] = \frac{2}{\pi} \int_0^\infty d\omega\, \frac{J(\omega)}{\omega} \cos\left[\omega\ (t - t')\right]$$

The spectral function

Fourier transform of the equation of motion for the environment variable

$$\tilde{q}_k(\omega) = -\frac{C_k}{m_k(\omega^2 - \omega_k^2)}\, \tilde{q}(\omega) \quad \Rightarrow \quad \chi_{env}(\omega) = -\sum_k \frac{C_k^2}{m_k(\omega^2 - \omega_k^2)}$$

or $\chi_{env}(\omega) = -\sum_k \left(\frac{C_k^2}{2m_k\omega_k(\omega\ +\ \omega_k)} - \frac{C_k^2}{2m_k\omega_k(\omega\ -\ \omega_k)} \right)$

Replacing $\omega \pm \omega_k \rightarrow \omega \pm \omega_k + i\epsilon$

and using $\dfrac{1}{(\omega \pm \omega_k) + i\epsilon} = \mathcal{P}\left(\dfrac{1}{\omega \pm \omega_k}\right) - i\pi\delta(\omega \pm \omega_k)$

we write $\mathrm{Im}\chi_{env}(\omega) \equiv \chi''_{env}(\omega) = \dfrac{\pi}{2}\sum_k \dfrac{C_k^2}{m_k\,\omega_k}[\delta(\omega - \omega_k) + \delta(\omega + \omega_k)]$

Or, for ω and $\omega_k > 0$ we have $J(\omega) = \chi''_{env}(\omega)$

Actually, $J(\omega) = \mathrm{Im}\mathcal{F}\left\{-i\,\theta\,(t - t')\left\langle\left[\sum_k C_k\,q_k(t)\,,\,\sum_{k'} C_{k'}\,q_{k'}(t')\right]\right\rangle\right\}$

Modelling the spectral function as $J(\omega) = \begin{cases} \eta\,\omega & \text{if } \omega < \Omega, \\ 0 & \text{if } \omega > \Omega, \end{cases}$

We rewrite

$$\sum_k \frac{C_k^2}{m_k\,\omega_k^2}\,\cos\left[\omega_k\,\left(t - t'\right)\right] = \frac{2}{\pi}\int_0^{\Omega} d\omega\,\eta\,\cos\left[\omega\,\left(t - t'\right)\right] = 2\,\eta\,\delta\left(t - t'\right),$$

and $\frac{d}{dt}\left\{\sum_k \frac{C_k^2}{m_k\,\omega_k^2}\int_0^t \cos\left[\omega_k\,\left(t - t'\right)\right]\,q(t')\,dt'\right\}.$ as

$$\frac{d}{dt}\int_0^t 2\,\eta\,\delta\left(t - t'\right)q(t')dt' = \eta\,\dot{q} + 2\,\eta\,\delta\left(t\right)q(0)$$

Bath force $$\tilde{f}(t) = \sum_k C_k \left\{ \frac{\dot{q}_k(0)}{\omega_k} \sin \omega_k t \,+\, q_k(0) \cos \omega_k t \right\}$$

Equilibrium position $\bar{q}_k \equiv C_k q(0)/m_k \omega_k^2$

Subtracting $\displaystyle\sum_k \frac{C_k^2 q(0)}{m_k \omega_k^2} \cos \omega_k t \;=\sum_k C_k \bar{q}_k \cos \omega_k t$ from both sides

cancels spurious term and generates

$$f(t) = \sum_k C_k \left\{ \frac{\dot{q}_k(0)}{\omega_k} \sin \omega_k t \,+\, (q_k(0) - \bar{q}_k) \cos \omega_k t \right\}$$

Equipartition theorem

$$\langle q_k(0) \rangle = \bar{q}_k \quad \text{and} \quad \langle \dot{q}_k(0) \rangle = \langle \dot{q}_k(0)\, \Delta q_k(0) \rangle = 0,$$

$$\langle \dot{q}_k(0)\, \dot{q}_{k'}(0) \rangle = \frac{k_B T}{m_k} \delta_{kk'},$$

$$\langle \Delta q_k(0)\, \Delta q_{k'}(0) \rangle = \frac{k_B T}{m_k \omega_k^2} \delta_{kk'}$$

Results in

$$M\,\ddot{q} + \eta\,\dot{q} + V'(q) = f(t)$$

$$\langle f(t) \rangle = 0,$$

$$\langle f(t)\, f(t') \rangle = 2\,\eta\, k_B\, T\, \delta\,(t - t')$$

Classical Langevin equation for the Brownian motion

In general $J(\omega) = \begin{cases} A_s \omega^s & \text{if} \quad \omega < \Omega \\ 0 & \text{if} \quad \omega > \Omega, \end{cases}$ $[A_s] = [M][T^{s-2}]$

$0 < s < 1$, *subohmic* case
$s = 1$, *ohmic* case
$1 < s$, *superohmic* case

Remark about this model

Alternative interaction $$\tilde{L}_I = \sum_k \tilde{C}_k \, q \, \dot{q}_k$$

Canonical momentum $$p_k = \frac{\partial L}{\partial \dot{q}_k} = m_k \, \dot{q}_k + \tilde{C}_k \, q$$

Hamiltonian $$\tilde{\mathcal{H}} = p \, \dot{q} + \sum_k p_k \, \dot{q}_k - L =$$

$$= \frac{p^2}{2\,M} + V(q) + \sum_k \left\{ \frac{1}{2\,m_k} \left(p_k - \tilde{C}_k \, q \right)^2 + \frac{1}{2} m_k \, \omega_k^2 \, q_k^2 \right\}$$

Under a canonical transformation

$$p \to p \;,\; q \to q \;,\; p_k \to m_k \, \omega_k \, q_k \;,\; q_k \to p_k / m_k \, \omega_k$$

and defining $C_k \equiv \tilde{C}_k \, \omega_k$

$$H \;=\; \frac{p^2}{2\,M} + V(q) + \sum_k C_k q_k q + \sum_k \left\{ \frac{p_k^2}{2\,m_k} + \frac{1}{2} m_k\,\omega_k^2\,q_k^2 \right\} + \sum_k \frac{C_k^2}{2 m_k \omega_k^2} q^2$$

Replacing $q_k \to C_k q_k / m_k\,\omega_k^2$ $\quad p_k \to m_k\,\omega_k^2\,p_k / C_k$

We can further write $\mathcal{H} = \frac{p^2}{2\,M} + V(q) + \sum_k \left\{ \frac{p_k^2}{2\,\mu_k} + \frac{1}{2}\mu_k\,\omega_k^2\,(q_k - q)^2 \right\}$

Where $\mu_k \equiv C_k^2 / m_k \omega_k^4$

and $J(\omega) = \frac{\pi}{2} \sum_k \mu_k\,\omega_k^3\,\delta\,(\omega - \omega_k)$

Final Remark : quantum Langevin equation

$$M\,\ddot{q} + \eta\,\dot{q} + V'(q) = f(t)$$

$$\langle f(t) \rangle = 0,$$

$$\frac{\langle \{\hat{f}(t), \hat{f}(t')\} \rangle}{2} = \frac{\hbar}{\pi} \int_0^\infty d\omega\,\eta\,\omega\ \coth\frac{\hbar\omega}{2k_B T}\cos\omega(t-t')$$

In the classical limit

$$\langle f(t)\, f(t') \rangle = 2\,\eta\,k_B\,T\,\delta\,(t-t')$$

Particle in general media: non-linear model

Dynamics in a continuum medium or of two Brownian particles; previous model not very appropriate. It needs generalization.

$$L_S = \frac{1}{2} M \dot{x}^2 \qquad L_R = \frac{1}{2} \sum_k m_k (\dot{R}_k \dot{R}_{-k} - \omega_k^2 R_k R_{-k}) \qquad L_I = \sum_k \tilde{C}_k(x) \dot{R}_k$$

Canonical transformation $\quad P_k \to m_k \omega_k R_k \qquad R_k \to P_k / m_k \omega_k$

$$\mathcal{H}_I = \frac{1}{2} \sum_k (C_{-k}(x) R_k + C_k(x) R_{-k}) - \sum_k \frac{C_k(x) C_{-k}(x)}{2 m_k \omega_k^2}$$

where $\quad C_k(x) \equiv \tilde{C}_k(x) \omega_k$

Translation invariant choice $\; C_k(x) = \kappa_k \, e^{ikx} \;$ makes counter-term constant

$$C_{-k}(x+d) R_k = C_{-k}(x) e^{-ikd} R_k \qquad \tilde{R}_k = e^{-ikd} R_k$$

Equation of motion $M\ddot{x} + \int_0^t K(x(t) - x(t'), t - t')\dot{x}(t')dt' = F(t)$

with $K(x, t) = \sum_k \frac{k^2 \kappa_k \kappa_{-k}}{m_k \omega_k^2} \cos kx \cos \omega_k t$

and $$F(t) = -\frac{\partial}{\partial x} \sum_k \left\{ \left(C_{-k}(x)\tilde{R}_k(0) + C_k(x)\tilde{R}_{-k}(0) \right) \frac{\cos \omega_k t}{2} + \left(C_{-k}(x)\dot{R}_k(0) + C_k(x)\dot{R}_{-k}(0) \right) \frac{\sin \omega_k t}{2\omega_k} \right\},$$

$\tilde{R}_k = R_k - C_k(x_0)/m_k \omega_k^2 \qquad C_k \equiv k\kappa_k$

then $K(x, t) = \sum_k \int_0^\infty d\omega 2k^2 \kappa_k \kappa_{-k} \frac{\mathrm{Im}\chi_k^{(0)}(\omega)}{\pi\omega} \cos k(x(t) - x(t')) \cos \omega(t - t')$

with $\mathrm{Im}\chi_k^{(0)}(\omega) = \pi\delta(\omega - \omega_k)/2m_k\omega_k$

With the replacement $\mathrm{Im}\chi_k^{(0)}(\omega) \to \mathrm{Im}\chi_k(\omega) = \dfrac{\gamma_k \omega}{m_k \left[\left(\omega^2 - \omega_k^2\right)^2 + \omega^2 \gamma_k^2 \right]},$

When $\omega \to 0$ we have $\mathrm{Im}\chi_k(\omega) \approx f(k)\omega\theta(\Omega - \omega)$

Then $M\ddot{x}(t) + \eta\dot{x}(t) = F(t)$ with $\eta \equiv \sum_k k^2 \kappa_k \kappa_{-k} f(k)$

and $\begin{cases} \langle F(t) \rangle = 0 \\ \langle F(t)F(t') \rangle = 2\eta k_B T \delta(t - t') \end{cases}$

Two Brownian particles $L_S = \dfrac{1}{2} M\dot{x}_1^2 + \dfrac{1}{2} M\dot{x}_2^2$

$$L_I = -\frac{1}{2} \sum_k \left[\left(C_{-k}(x_1) + C_{-k}(x_2) \right) R_k + \left(C_k(x_1) + C_k(x_2) \right) R_{-k} \right]$$

Equations of motion

$$M\ddot{x}_i + \int_0^t K(x_i(t) - x_i(t'), t - t')\dot{x}_i(t')dt' + \int_0^t K(x_i(t) - x_j(t'), t - t')\dot{x}_j(t')dt' + \frac{\partial(V(x_i(t) - x_j(t)))}{\partial x_i} = F_i(t)$$

Effective potential $V(r(t)) = -\sum_k \int_0^\infty d\omega 2\kappa_k\kappa_{-k} \frac{\mathrm{Im}\chi_k^{(0)}(\omega)}{\pi\omega} \cos kr(t)$

We can further define $\eta g(k) \equiv \sum_{k'} \kappa_{k'}\kappa_{-k'} f(k')\delta(k - k')$

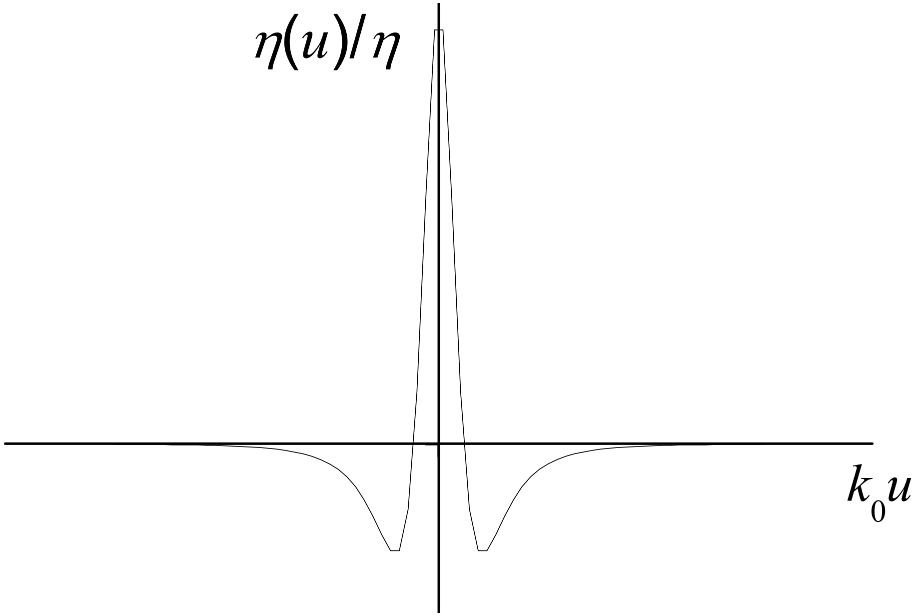
with $\int_0^\infty g(k)k^2 dk = 1$ and model $g(k) = Ae^{-k/k_0}$ where $A = 1/(2k_0^3)$

Applying all this to $K(x,t) = \sum_k \frac{k^2\kappa_k\kappa_{-k}}{m_k\omega_k^2} \cos kx \cos\omega_k t$

$$K(x_1(t) - x_2(t'), t - t') = 2\delta(t - t')\eta(u(t)) \qquad \text{for} \qquad u(t) = x_1(t) - x_2(t)$$

$$\eta(u(t)) = \eta\left(\frac{1}{(k_0^2u^2+1)^2} - \frac{4u^2k_0^2}{(k_0^2u^2+1)^3}\right) \qquad \text{and} \qquad V(u(t)) = -\frac{2\Omega\eta}{\pi k_0^2\,(k_0^2u^2(t)+1)}$$

$$\langle F_1(t)F_2(t')\rangle = 2\eta(u(t))k_BT\delta(t - t')$$



Equations of motion

$$M\ddot{u}(t) + \eta\dot{u}(t) - \eta(u(t))\dot{u} + V'(u(t)) = F_u(t) \qquad F_u(t) = F_1(t) - F_2(t)$$

$$M\ddot{q}(t) + \eta\dot{q}(t) + \eta(u(t))\dot{q} = F_q(t) \qquad F_q(t) = (F_1(t) + F_2(t))/2$$

$$\langle F_u(t)\rangle = 0 \quad \text{and} \quad \langle F_u(t)F_u(t')\rangle = 4k_BT(\eta - \eta(u))\delta(t-t')$$
$$\langle F_q(t)\rangle = 0 \quad \text{and} \quad \langle F_q(t)F_q(t')\rangle = k_BT(\eta + \eta(u))\delta(t-t')$$

For the C.M. : particle of mass $2M$

For the relative coordinate : particle of mass $M/2$

Collision model

Manifestly translation invariant form

$$\mathcal{H}(q,p,q_i,p_i) = \frac{p^2}{2M} + V(q) + \sum_{i=1}^{N} U(q_i - q) + \sum_{i=1}^{N} \frac{p_i^2}{2m}$$

Canonical transformation (translation)

$$q_i - q \to Q_i \qquad p + \sum_i p_i \to P$$

$$\mathcal{H}'(q,P,Q_i,p_i) = \frac{1}{2M}\left(P - \sum_{i=1}^{N} p_i\right)^2 + V(q) + \sum_{i=1}^{N}\left(\frac{p_i^2}{2m} + U(Q_i)\right)$$

Equations of motion

$$M\ddot{q} + V'(q) - \sum_{i=1}^{N} U'(q_i - q) = 0$$

and $\qquad m\ddot{q}_i + U'(q_i - q) = 0$

Other environmental models

Rotating wave approximation (RWA)

Genuine quantum model

$$\mathcal{H}_{RWA} = \hbar\omega_a a^\dagger a + \sum_k \{V_k a^\dagger b_k + V_k^* a\, b_k^\dagger\} + \sum_k \hbar\omega_k b_k^\dagger b_k$$

where
$$\begin{cases} a = \sqrt{\dfrac{M\omega_a}{2\hbar}}\left(q + i\dfrac{p}{M\omega_a}\right) \text{ and} \\ b_k = \sqrt{\dfrac{m_k\omega_k}{2\hbar}}\left(q_k + i\dfrac{p_k}{m_k\omega_k}\right) \end{cases}$$

and define
$$S(\omega) = \frac{2\pi}{\hbar^2}\sum_k |V_k|^2 \delta(\omega - \omega_k)$$

Relation to the other spectral function

$$V_k = \hbar C_k / 2\sqrt{M\,\omega_a\, m_k\, \omega_k} \quad \Longrightarrow \quad J(\omega) = M S(\omega)\omega_a$$

$$S(\omega) \approx S(\omega_a) = 2\gamma \qquad n(\omega) \approx n(\omega_a) \qquad n(\omega) = \frac{1}{\exp\left(\frac{\hbar\,\omega}{k_B T}\right) - 1}$$

Fermi's golden rule $\quad w = 2\gamma = \frac{2\pi}{\hbar^2} \sum_{k \neq a} |V_k|^2 \delta(\omega_a - \omega_k) = \frac{2\pi}{\hbar^2} |V_a|^2 \rho(\omega_a)$

Two state system (TSS) bath

$$\mathcal{H}_{TSS} = \mathcal{H}_0 + \mathcal{H}_I + \mathcal{H}_R$$

$$\sigma_k^{(+)} = [\sigma_k^{(-)}]^\dagger \equiv \frac{\sigma_k^{(x)} + i\,\sigma_k^{(y)}}{2} \qquad \begin{cases} \mathcal{H}_I = -\sum_k F_k\, q\, \sigma_k^{(x)}, \\ \mathcal{H}_R = \sum_k \hbar\,\omega_k\, \sigma_k^{(z)} \end{cases}$$

$$q_k = \sqrt{\frac{\hbar}{2m_k\omega_k}}\left(b_k + b_k^\dagger\right) = \sqrt{\frac{\hbar}{2m_k\omega_k}}\left(\sigma_k^{(-)} + \sigma_k^{(+)}\right) = \sqrt{\frac{\hbar}{2m_k\omega_k}}\sigma_k^{(x)}$$

$$F_k = \sqrt{\frac{\hbar}{2m_k\omega_k}}C_k \qquad J_{TSS}(\omega) \equiv \pi \sum_k F_k^2 \qquad J_{TSS}(\omega) = \hbar J(\omega)$$

Jaynes-Cummings model (JC): RWA of the TSS

$$\mathcal{H}_I = -\sum_k \left(G_k\sigma_k^{(+)}\,a + G_k^*\sigma_k^{(-)}\,a^\dagger\right) \qquad G_k = \sqrt{\frac{\hbar}{2M\omega_a}}\,F_k$$

$$S_{JC}(\omega) \equiv \pi \sum_k G_k^2\,\delta(\omega - \omega_k)$$

$$S_{JC}(\omega) = \frac{\hbar}{2M\omega_a}J_{TSS}(\omega) = \frac{\hbar^2}{2M\omega_a}J(\omega)$$