14.3: The Dynamic Friction Kernel

The convolution integral term

$$\int_0^t d\tau\ \dot{q}(\tau)\zeta(t-\tau)$$

is called the **memory integral** because it depends, in general, on the entire history of the evolution of q. Physically it expresses the fact that the bath requires a finite time to respond to any fluctuation in the motion of the system (q). This, in turn, affects how the bath acts back on the system. Thus, the force that the bath exerts on the system presently depends on what the system coordinate q did in the past. However, we have seen previously the regression of fluctuations (their decay to 0) over time. Thus, we expect that what the system did very far in the past will no longer the force it feels presently, i.e., that the lower limit of the memory integral (which is rigorously 0) could be replaced by $t - t_{\text{mem}}$, where t_{mem} is the maximum time over which memory of what the system coordinate did in the past is important. This can be interpreted as a indicating a certain decay time for the friction kernel $\zeta(t)$. In fact, $\zeta(t)$ often does decay to 0 in a relatively short time. Often this decay takes the form of a rapid initial decay followed by a slow final decay, as shown in the figure below:

Consider the extreme case that the bath is capable of responding infinitely quickly to changes in the system coordinate q. This would be the case, for example, if there were a large mass disparity between the system and the bath ($m \gg m_\alpha$). Then, the bath retains *no* memory of what the system did in the past, and we could take $\zeta(t)$ to be a δ-function in time:

$$\zeta(t) = 2\zeta_0\delta(t)$$

Then

$$\int_0^t d\tau\ \dot{q}(\tau)\zeta(t-\tau) = \int_0^t d\tau \dot{q}(t-\tau)\zeta(\tau) = 2\zeta_0 \int_0^t d\tau\ \delta(\tau)\dot{q}(t-\tau) = \zeta_0\dot{q}(t)$$

and the GLE becomes

$$m\ddot{q} = -\frac{\partial\phi}{\partial q} - \zeta_0\dot{q} + R(t)$$

This simpler equation of motion is known as the **Langevin equation** and it is clearly a special case of the more generalized equation of motion. It is often invoked to describe Brownian motion where clearly such a mass disparity is present. The constant ζ_0 is known as the static friction and is given by

$$\zeta_0 = \int_0^\infty dt\ \zeta(t)$$

In fact, this is a general relation for determining the static friction constant.

The other extreme is a very sluggish bath that responds slowly to changes in the system coordinate. In this case, we may take $\zeta(t)$ to be a constant $\zeta \equiv \zeta(0)$, at least, for times short compared to the response time of the bath. Then, the memory integral becomes

$$\int_0^t d\tau\ \dot{q}(\tau)\zeta(t-\tau) \approx \zeta(q(t) - q(0))$$

and the GLE becomes

$$m\ddot{q} = -\frac{\partial}{\partial q}\left(\phi(q) + \frac{1}{2}\zeta(q-q_0)^2\right) + R(t)$$

where the friction term now manifests itself as an extra harmonic term added to the potential. Such a term has the effect of trapping the system in certain regions of configuration space, an effect known as **dynamic caging**. An example of this is a dilute mixture of small, light particles in a bath of heavy, large particles. The light particles can get trapped in regions of space where many bath particles are in a sort of spatial 'cage." Only the rare fluctuations in the bath that open up larger holes in configuration space allow the light particles to escape the cage, occasionally, after which, they often get trapped again in a new cage for a similar time interval.