14.5: Derivation of the GLE

The GLE can be derived from the harmonic bath Hamiltonian by simply solving Hamilton's equations of motion, which take the form

$$\dot{q} = \frac{P}{m}$$

$$\dot{p} = -\frac{\partial \phi}{\partial q} - \sum_\alpha g_\alpha x_\alpha - \sum_\alpha \frac{g_\alpha^2}{m_\alpha \omega_\alpha^2} q$$

$$\dot{x}_\alpha = \frac{P_\alpha}{m_\alpha}$$

$$\dot{p}_\alpha = -m_\alpha \omega_\alpha^2 x_\alpha - g_\alpha q$$

This set of equations can also be written as second order differential equation:

$m\ddot{q}$	=	$-\frac{\partial \phi}{\partial q} - \sum_\alpha g_\alpha x_\alpha - \sum_\alpha \frac{g_\alpha^2}{m_\alpha \omega_\alpha^2} q$
$m_\alpha \ddot{x}_\alpha$	=	$-m_\alpha \omega_\alpha^2 x_\alpha - g_\alpha q$

In order to derive an equation for q, we solve explicitly for the dynamics of the bath variables and then substitute into the equation for q. The equation for x_α is a second order inhomogeneous differential equation, which can be solved by Laplace transforms. We simply take the Laplace transform of both sides. Denote the Laplace transforms of q and x_α as

$\tilde{q}(s)$	=	$\int_0^\infty dt\ e^{-st} q(t)$
$\tilde{x}_\alpha$	=	$\int_0^\infty dt\ e^{-st} x_\alpha(t)$

and recognizing that

$$\int_0^\infty dt\ e^{-st} \ddot{x}_\alpha(t) = s^2 \tilde{x}_\alpha(s) - s x_\alpha(0) - \dot{x}_\alpha(0)$$

we obtain the following equation for $\tilde{x}_\alpha(s)$:

$$(s^2 + \omega_\alpha^2)\tilde{x}_\alpha(s) = s x_\alpha(0) + \dot{x}_\alpha(0) - \frac{g_\alpha}{m_\alpha} \tilde{q}(s)$$

or

$$\tilde{x}_\alpha(s) = \frac{s}{s^2 + \omega_\alpha^2} x_\alpha(0) + \frac{1}{s^2 + \omega_\alpha^2} \dot{x}_\alpha(0) - \frac{g_\alpha}{m_\alpha} \frac{\tilde{q}(s)}{s^2 + \omega_\alpha^2}$$

$x_\alpha(t)$can be obtained by inverse Laplace transformation, which is equivalent to a contour integral in the complex s-plane around a contour that encloses all the poles of the integrand. This contour is known as the *Bromwich* contour. To see how this works, consider the first term in the above expression. The inverse Laplace transform is

$$\frac{1}{2\pi i} \oint ds\ \frac{s e^{st}}{s^2 + \omega_\alpha^2} = \frac{1}{2\pi i} \oint ds\ \frac{s e^{st}}{(s + i\omega_\alpha)(s - i\omega_\alpha)}$$

The integrand has two poles on the imaginary s-axis at $\pm i\omega_\alpha$. Integration over the contour that encloses these poles picks up both residues from these poles. Since the poles are simple poles, then, from the residue theorem:

$$\frac{1}{2\pi i} \oint ds\ \frac{s e^{st}}{(s + i\omega_\alpha)(s - i\omega_\alpha)} = \frac{1}{2\pi i} \left[2\pi i \left(\frac{i\omega_\alpha e^{i\omega_\alpha t}}{2i\omega_\alpha} + \frac{-i\omega_\alpha e^{i\omega_\alpha t}}{-2i\omega_\alpha} \right) \right] = \cos \omega_\alpha t$$

By the same method, the second term will give $(\sin \omega_\alpha t)/\omega_\alpha$. The last term is the inverse Laplace transform of a product of $q(S)\tilde{q}(s)$ and $1/(s^2 + \omega_\alpha^2)$. From the convolution theorem of Laplace transforms, the Laplace transform of a convolution gives the product of Laplace transforms:

$$\int_0^\infty dt\ e^{-st} \int_0^t d\tau\ f(\tau)g(t-\tau) = \tilde{f}(s)\tilde{g}(s)$$

Thus, the last term will be the convolution of $q(t)$ with $(\sin\omega_\alpha t)/\omega_\alpha$. Putting these results together, gives, as the solution for $x_\alpha(t)$:

$$x_\alpha(t) = x_\alpha(0)\cos\omega_\alpha t + \frac{\dot{x}_\alpha(0)}{\omega_\alpha}\sin\omega_\alpha t - \frac{g_\alpha}{m_\alpha\omega_\alpha}\int_0^t d\tau q(\tau)\sin\omega_\alpha(t-\tau)$$

The convolution term can be expressed in terms of $\dot{q}$ rather than q by integrating it by parts:

$$\frac{g_\alpha}{m_\alpha\omega_\alpha}\int_0^t d\tau\ q(\tau)\sin\omega_\alpha(t-\tau) = \frac{g_\alpha}{m_\alpha\omega_\alpha^2}\left[q(t) - q(0)\cos\omega_\alpha t\right] - \frac{g_\alpha}{m_\alpha\omega_\alpha^2}\int_0^t d\tau\ \dot{q}(\tau)\cos\omega_\alpha(t-\tau)$$

The reasons for preferring this form will be made clear shortly. The bath variables can now be seen to evolve according to

$$x_\alpha(t) = x_\alpha(0)\cos\omega_\alpha t + \frac{\dot{x}(0)}{\omega_\alpha}\sin\omega_\alpha t + \frac{g_\alpha}{m_\alpha\omega_\alpha^2}\int_0^t d\tau\ \dot{q}(\tau)\cos\omega_\alpha(t-\tau) - \frac{g_\alpha}{m_{alpha}\omega_\alpha^2}\left[q(t) - q(0)\cos\omega_\alpha t\right]$$

Substituting this into the equation of motion for q, we find

$$m\ddot{q} = -\frac{\partial\phi}{\partial q} - \sum_\alpha g_\alpha\left[x_\alpha(0)\cos\omega_\alpha t + \frac{P_\alpha(0)}{m_\alpha\omega_\alpha}\sin\omega_\alpha t + \frac{g_\alpha}{m_\alpha\omega_\alpha^2}q(0)\cos\omega_\alpha t\right] - \sum_\alpha\frac{g_\alpha^2}{m_\alpha\omega_\alpha^2}\int_0^t d\tau\dot{q}(\tau)\cos\omega_\alpha(t-\tau)$$

$+\sum_\alpha \frac{g_\alpha^2}{m_\alpha\omega_\alpha^2}q(t) - \sum_\alpha \frac{g_\alpha^2}{m_\alpha\omega_\alpha^2}q(t)$

We now introduce the following notation for the sums over bath modes appearing in this equation:

1.

Define a dynamic *friction kernel*

$$\zeta(t) = \sum_\alpha \frac{g_\alpha}{m_\alpha\omega_\alpha^2}\cos\omega_\alpha t$$

2.

Define a *random force*

$$R(t) = -\sum_\alpha g_\alpha\left[\left(x_\alpha(0) + \frac{g_\alpha}{m_\alpha\omega_\alpha^2}q(0)\right)\cos\omega_\alpha t + \frac{P_\alpha(0)}{m_\alpha\omega_\alpha}\sin\omega_\alpha t\right]$$

Using these definitions, the equation of motion for q reads

$$m\ddot{q} = -\frac{\partial\phi}{\partial q} - \int_0^t d\tau\ \dot{q}(\tau)\zeta(t-\tau) + R(t) \qquad (1)$$

Eq. (1) is known as the *generalized Langevin equation*. Note that it takes the form of a one-dimensional particle subject to a potential $\phi(q)$, driven by a forcing function $R(t)$ and with a nonlocal (in time) damping term $-\int_0^t d\tau\ \dot{q}(\tau)\zeta(t-\tau)$, which depends, in general, on the entire history of the evolution of q. The GLE is often taken as a phenomenological equation of motion for a coordinate q coupled to a general bath. In this spirit, it is worth taking a moment to discuss the physical meaning of the terms appearing in the equation.