V.3.3 Caldeira–Leggett model

In this subsection, we introduce a simple microscopical model for the fluid in which the Brownian particle is immersed, which leads to a friction force proportional to the velocity.

V.3.3 a Caldeira–Leggett Hamiltonian

Consider a "Brownian" particle of mass M, with position and momentum $x(t)$ and $p(t)$ respectively, interacting with a "bath" of N mutually independent harmonic oscillators with respective masses m_j, positions $x_j(t)$ and momenta $p_j(t)$. The coupling between the particle and each of the oscillators is assumed to be bilinear in their positions, with a coupling strength C_j. Additionally, we also allow for the Brownian particle to be in a position-dependent potential $V_0(x)$.

Under these assumptions, the Hamilton function of the system consisting of the Brownian particle and the oscillators reads

$$H = \frac{p^2}{2M} + V_0(x) + \sum_{j=1}^{N}\left(\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 x_j^2\right) - \sum_{j=1}^{N} C_j\, x_j\, x. \tag{V.68a}$$

It is convenient to rewrite the potential V_0 as

$$V_0(x) = V(x) + \left(\sum_{j=1}^{N}\frac{C_j^2}{2m_j\omega_j^2}\right)x^2,$$

where the second term in the right member clearly vanishes when the Brownian particle does not couple to the oscillators. The Hamilton function (V.68a) can then be recast as

$$H = \frac{p^2}{2M} + V(x) + \sum_{j=1}^{N}\left[\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2\left(x_j - \frac{C_j}{m_j\omega_j^2}\,x\right)^2\right]. \tag{V.68b}$$

This Hamilton function—or its quantum-mechanical counterpart, which we shall meet again in Sec. VI.4.3 c—is known as the *Caldeira*[(bm)]*–Leggett*[(bn)] *Hamiltonian* [46].

For a physical interpretation, it is interesting to rescale the characteristics of the bath oscillators, performing the change of variables

$$m_j \to m'_j = \frac{m_j}{\lambda_j^2}, \qquad x_j \to x'_j = \lambda_j x_j, \qquad p_j \to p'_j = \frac{p_j}{\lambda_j}, \qquad j = 1,\dots,N$$

with $\lambda_j \equiv \dfrac{m_j\omega_j^2}{C_j}$ dimensionless constants. The Hamiltonian (V.68b) then becomes

$$H = \frac{p^2}{2M} + V(x) + \sum_{j=1}^{N}\left[\frac{p_j'^2}{2m'_j} + \frac{1}{2}m'_j\omega_j^2\left(x'_j - x\right)^2\right], \tag{V.69}$$

i.e. the interaction term between the Brownian particle and each oscillator only depends on their relative distance. The Caldeira–Leggett Hamiltonian can thus be interpreted as that of a particle of mass m, moving in the potential V with (light) particles of masses m'_j attached to it by springs of respective spring constants $m'_j\omega_j^2$ [47].

(bm) A. Caldeira, born 1950 (bn) A. J. Leggett, born 1938

Coming back to the form (V.68b) of the Hamilton function, the corresponding equations of motion, derived from the Hamilton equations (II.1), read

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \frac{1}{M}\,p(t), \qquad \frac{\mathrm{d}p(t)}{\mathrm{d}t} = \sum_{j=1}^{N} C_j\left[x_j(t) - \frac{C_j}{m_j\omega_j^2}\,x(t)\right] - \frac{\mathrm{d}V\big(x(t)\big)}{\mathrm{d}x}, \tag{V.70a}$$

$$\frac{\mathrm{d}x_j(t)}{\mathrm{d}t} = \frac{1}{M}\,p_j(t), \qquad \frac{\mathrm{d}p_j(t)}{\mathrm{d}t} = -m\omega_j^2 x_j(t) + C_j x(t), \tag{V.70b}$$

which can naturally be recast as second-order differential equations for the positions $x(t)$, $x_j(t)$.

V.3.3 b Free particle

Let us now assume that the Brownian particle is "free", in the sense that the potential V in the Hamiltonian (V.68b) vanishes, $V(x) = 0$. In that case, the last term on the right-hand side of second equation of motion for the Brownian particle, Eq. (V.70a), vanishes.

Integrating formally the equations of motion (V.70b) for each oscillator between an initial time t_0 and time t, one obtains

$$x_j(t) = x_j(t_0)\cos\omega_j(t-t_0) + \frac{p_j(t_0)}{m_j\omega_j}\sin\omega_j(t-t_0) + C_j\int_{t_0}^{t} x(t')\,\frac{\sin\omega_j(t-t')}{m_j\omega_j}\,\mathrm{d}t'.$$

Performing an integration by parts and rearranging the terms, one finds

$$x_j(t) - \frac{C_j}{m_j\omega_j^2}\,x(t) = \left[x_j(t_0) - \frac{C_j}{m_j\omega_j^2}\,x(t_0)\right]\cos\omega_j(t-t_0) + \frac{p_j(t_0)}{m_j\omega_j}\sin\omega_j(t-t_0) - C_j\int_{t_0}^{t}\frac{p(t')}{M}\,\frac{\cos\omega_j(t-t')}{m_j\omega_j^2}\,\mathrm{d}t'.$$

This can then be inserted in the right member of the second equation of motion in Eq. (V.70a). Combining with the first equation of motion giving $p(t)$ in function of $\mathrm{d}x(t)/\mathrm{d}t$, one obtains

$$\frac{\mathrm{d}^2x(t)}{\mathrm{d}t^2} + \int_{t_0}^{t}\left[\frac{1}{M}\sum_{j=1}^{N}\frac{C_j^2}{m_j\omega_j^2}\cos\omega_j(t-t')\right]\frac{\mathrm{d}x(t')}{\mathrm{d}t}\,\mathrm{d}t' = \frac{1}{M}\sum_{j=1}^{N}C_j\left[x_j(t_0)\cos\omega_j(t-t_0) + \frac{p_j(t_0)}{m_j\omega_j}\sin\omega_j(t-t_0)\right] - \left[\frac{1}{M}\sum_{j=1}^{N}\frac{C_j^2}{m_j\omega_j^2}\cos\omega_j(t-t_0)\right]x(t_0). \tag{V.71}$$

Introducing the quantities

$$\gamma(t) \equiv \frac{1}{M}\sum_{j=1}^{N}\frac{C_j^2}{m_j\omega_j^2}\cos\omega_j t \tag{V.72a}$$

and

$$F_{\mathrm{L}}(t) \equiv \sum_{j=1}^{N}C_j\left[x_j(t_0)\cos\omega_j(t-t_0) + \frac{p_j(t_0)}{m_j\omega_j}\sin\omega_j(t-t_0)\right], \tag{V.72b}$$

which both only involve characteristics of the bath, Eq. (V.71) becomes

$$M\frac{\mathrm{d}^2x(t)}{\mathrm{d}t^2} + M\int_{t_0}^{t}\gamma(t-t')\,\frac{\mathrm{d}x(t')}{\mathrm{d}t}\,\mathrm{d}t' = -M\gamma(t-t_0)x(t_0) + F_{\mathrm{L}}(t). \tag{V.72c}$$

This evolution equation for the position—or equivalently the velocity, since $x(t_0)$ in the right-hand side is only a number—of the Brownian particle is exact, and follows from the Hamiltonian equations of motion without any approximation. It is obviously very reminiscent of the generalized Langevin equation (V.61a), up to a few points, namely the lower bound of the integral, the term $-M\gamma(t-t_0)x(t_0)$, and the question whether $F_{\mathrm{L}}(t)$ as defined by relation (V.72b) is a Langevin force.

The first two differences between Eq. (V.61a) and Eq. (V.72c), rewritten in terms of the velocity, are easily dealt with, by sending the arbitrary initial time t_0 to $-\infty$: anticipating on what we shall find below, the memory kernel $\gamma(t)$ vanishes at infinity for the usual choices for the distribution of the bath oscillator frequencies, which suppresses the contribution $-M\gamma(t-t_0)x(t_0)$.

In turn, the characteristics of the force $F_{\rm L}(t)$, Eq. (V.72b), depend on the initial positions and momenta $\{x_j(t_0), p_j(t_0)\}$ of the bath oscillators at time t_0. Strictly speaking, if the latter are exactly known, then $F_{\rm L}(t)$ is a deterministic force, rather than a fluctuating one. When the number N of oscillators becomes large, the deterministic character of the force becomes elusive, since in practice one cannot know the variables $\{x_j(t_0), p_j(t_0)\}$ with infinite accuracy (see the discussion in Sec. II.1). In practice, it is then more fruitful to consider the phase-space density $\rho_N\big(t_0, \{q_j\}, \{p_j\}\big)$, Eq. (II.3). Assuming that at t_0 the bath oscillators are in thermal equilibrium at temperature T, ρ_N at that instant is given by the canonical distribution

$$\rho_N\big(t_0, \{q_j\}, \{p_j\}\big) = \frac{1}{Z_N(T)} \exp\left[-\frac{1}{k_BT}\sum_{j=1}^{N}\left(\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 x_j^2\right)\right].$$

Computing average values with this Gaussian distribution,[68] one finds that the force $F_{\rm L}(t)$ as given by Eq. (V.72b) is a stationary Gaussian random process, with vanishing average value $\langle F_{\rm L}(t)\rangle = 0$ and the autocorrelation function

$$\langle F_{\rm L}(t) F_{\rm L}(t+\tau)\rangle = Mk_BT\gamma(\tau).$$

That is, $F_{\rm L}(t)$ has the properties of a Langevin force as discussed in § V.1.1 b.

Remark: For $V(x) = 0$, the Hamilton function (V.69) is invariant under global translations of all (Brownian and light) particles, since it only depends on relative distances. As a consequence, the corresponding total momentum $p + \sum_j p'_j$ is conserved.

V.3.3 c Limiting case of a continuous bath

As long as the number N of bath oscillators is finite, the Caldeira–Leggett Hamiltonian (V.68b) with $V(x) = 0$ [or with a harmonic potential $V(x) \propto x^2$] strictly speaking leads to a periodic dynamical evolution. As thus, it cannot provide an underlying microscopic model for Brownian motion.[69] The latter can however emerge if one considers the limit of an infinite number of bath degrees of freedom,[70] in particular if the oscillator frequencies span a continuous interval.

To provide an appropriate description for both finite- and infinite-N cases, it is convenient to introduce the *spectral density of the coupling to the bath*

$$J(\omega) \equiv \frac{\pi}{2}\sum_j \frac{C_j^2}{m_j\omega_j}\,\delta(\omega-\omega_j). \tag{V.73}$$

With its help, the memory kernel (V.72a) can be recast as

$$\gamma(t) = \frac{2}{\pi}\int \frac{J(\omega)}{M\omega}\cos\omega t\,{\rm d}\omega. \tag{V.74}$$

[68] As noted in the remark at the end of Sec. V.1.1 b, this is indeed the meaning of expectation values in this chapter, since we are averaging over all microscopic configurations $\{x_j(t_0), p_j(t_0)\}$ compatible with a given macroscopic temperature.

[69] ... valid on any time scale. Physically, if $N \gg 1$, the Poincaré[bo] recurrence time of the system will in general be very large. On a time scale much smaller than this recurrence time, the periodicity of the problem can be ignored, and the dynamics is well described by the generalized Langevin model.

[70] The frequencies of the bath oscillators should not stand in simple relation to each other—as for instance if they were all multiples of a single frequency.

[bo] H. Poincaré, 1854–1912

If N is finite, then $J(\omega)$ is a discrete sum of δ-distributions. Let ε denote the typical spacing between two successive frequencies ω_j of the bath oscillators. For evolutions on time scales much smaller than $1/\varepsilon$, the discreteness of the set of frequencies may be ignored.(69) Consider the continuous function $J_c(\omega)$, such that on every interval $\mathcal{I}_\omega \equiv [\omega, \omega + \mathrm{d}\omega]$ of width $\mathrm{d}\omega \gg \varepsilon$, with $\mathrm{d}\omega$ small enough that $J_c(\omega)$ does not vary significantly over $\mathcal{I}_\omega$, one has

$$J_c(\omega)\,\mathrm{d}\omega = \sum_{\omega_j \in \mathcal{I}_\omega} \frac{\pi}{2} \frac{C_j^2}{m_j \omega_j}. \tag{V.75}$$

One can then replace $J(\omega)$ by $J_c(\omega)$, for instance in Eq. (V.74), which amounts to considering a continuous spectrum of bath frequencies.

The simplest possible choice for $J_c(\omega)$ consists in assuming that it is proportional to the frequency for positive values of ω. To be more realistic, one also introduces an upper cutoff frequency ω_c, above which J_c vanishes:

$$J_c(\omega) = \begin{cases} M\gamma\omega & \text{for } 0 \leq \omega \leq \omega_c, \\ 0 & \text{otherwise.} \end{cases} \tag{V.76}$$

This choice leads at once with Eq. (V.74) to $\gamma(t) = 2\gamma\delta_{\omega_c}(t)$, where

$$\delta_{\omega_c}(t) = \frac{1}{\pi} \frac{\sin \omega_c t}{t} \tag{V.77}$$

is a function that tends to $\delta(t)$ as $\omega_c \to +\infty$ and only takes significant values on a range of typical width ω_c^{-1} around $t = 0$. ω_c^{-1} is thus the characteristic time scale of the memory kernel $\gamma(t)$.

Remarks:

∗ In the limit $\omega_c \to +\infty$, i.e. of an instantaneous memory kernel $\gamma(t) = 2\gamma\delta(t)$, the evolution equation (V.72c) reduces to the Langevin equation [cf. (V.1)] $M\ddot{x}(t) + M\gamma\dot{x}(t) = F_{\mathrm{L}}(t)$. As this is also the equation governing the electric charge in a RL circuit, the choice $J_c(\omega) \propto \omega$ at low frequencies is referred to as "ohmic bath". In turn, a harmonic bath characterized by $J_c(\omega) \propto \omega^\eta$ with $\eta < 1$ (resp. $\eta > 1$) is referred to as sub-ohmic (resp. super-ohmic).(71)

∗ Instead of a step function $\Theta(\omega_c - \omega)$ as in Eq. (V.76), one may also use a smoother cutoff function to handle the ultraviolet modes in the bath, without affecting the physical results significantly.

(71)See Ref. [48] for a study in the non-ohmic case.