VI.4.3 d Caldeira–Leggett model

In the previous paragraph, we have seen that the phenomenological Langevin model for the motion of a Brownian particle submitted to an external force yields correlation functions which do not fulfill the sum rules of linear-response theory. This means that the model can actually not be the macroscopic manifestation of an underlying microscopic dynamical model.[88]

From Sec. V.3.3, we already know that a classical heavy particle interacting with a bath of classical independent harmonic oscillators—which constitutes a special case of the model introduced in § VI.4.3 a—actually obeys a generalized Langevin equation when the bath degrees of freedom are integrated out. Here we want to consider this model again, now in the quantum-mechanical case.

Since the dynamics along different directions decouple, we restrict the study to a one-dimensional system, whose Hamilton operator is given by [cf. Eq. (V.68b)]

$$\hat{H}_0 = \frac{\hat{p}^2}{2M} + \sum_{j=1}^{N}\left[\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2\left(\hat{x}_j - \frac{C_j}{m_j\omega_j^2}\hat{x}\right)^2\right]. \tag{VI.107}$$

$\hat{x}$, $\hat{p}$, M are the position, momentum and mass of the heavy particle, while $\hat{x}_j$, $\hat{p}_j$ and m_j denote those of the harmonic oscillators, with resonant frequencies ω_j, with which the particle interacts.

Equations of motion

The Heisenberg equation (II.37) for the position and momentum of the heavy particle read

$$\frac{\mathrm{d}\hat{x}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\big[\hat{x}(t), \hat{H}_0\big] = \frac{1}{M}\hat{p}(t), \tag{VI.108a}$$

$$\frac{\mathrm{d}\hat{p}(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\big[\hat{p}(t), \hat{H}_0\big] = \sum_{j=1}^{N} C_j\hat{x}_j(t) - \left(\sum_{j=1}^{N}\frac{C_j^2}{m_j\omega_j^2}\right)\hat{x}(t). \tag{VI.108b}$$

These equations are sometimes referred to as *Heisenberg–Langevin equations*.

The first term on the right hand side of the evolution equation for the momentum only depends on the bath degrees of freedom. Introducing the ladder operators $\hat{a}_j(t)$, $\hat{a}_j^\dagger(t)$ of the bath oscillators, it can be rewritten as

$$\hat{R}(t) \equiv \sum_{j=1}^{N} C_j\hat{x}_j(t) = \sum_{j=1}^{N} C_j\sqrt{\frac{\hbar}{2m_j\omega_j}}\Big[\hat{a}_j(t) + \hat{a}_j^\dagger(t)\Big]. \tag{VI.109}$$

The Heisenberg equation

$$\frac{\mathrm{d}\hat{a}_j(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\big[\hat{a}_j(t), \hat{H}_0\big] = -\mathrm{i}\omega_j\hat{a}_j(t) + \mathrm{i}\frac{C_j}{\sqrt{2\hbar m_j\omega_j}}\hat{x}(t)$$

obeyed by the annihilation operator for the j-th oscillator admits the solution

$$\hat{a}_j(t) = \hat{a}_j(t_0)\,\mathrm{e}^{-\mathrm{i}\omega_j(t-t_0)} + \mathrm{i}\frac{C_j}{\sqrt{2\hbar m_j\omega_j}}\int_{t_0}^{t}\hat{x}(t')\,\mathrm{e}^{-\mathrm{i}\omega_j(t-t')}\,\mathrm{d}t',$$

with t_0 an arbitrary initial time. Inserting this expression and its adjoint in Eq. (VI.109), the evolution equation (VI.108b) becomes

$$\frac{\mathrm{d}\hat{p}(t)}{\mathrm{d}t} = \sum_{j=1}^{N}\frac{C_j^2}{2m_j\omega_j}\left[\mathrm{i}\int_{t_0}^{t}\hat{x}(t')\,\mathrm{e}^{-\mathrm{i}\omega_j(t-t')}\,\mathrm{d}t' + \text{h.c.}\right] + \hat{F}_{\mathrm{L}}(t) - \left(\sum_{j=1}^{N}\frac{C_j^2}{m_j\omega_j^2}\right)\hat{x}(t), \tag{VI.110a}$$

where the operator $\hat{F}_{\mathrm{L}}(t)$ is defined as

[88] More precisely, the Langevin equation cannot emerge as macroscopic limit valid on arbitrary time scales—or equivalently for all frequencies—of an underlying microscopic theory, although it might constitute an excellent approximation in a limited time / frequency range.

$$\hat{F}_{\rm L}(t) \equiv \sum_{j=1}^{N} C_j \sqrt{\frac{\hbar}{2m_j\omega_j}} \Big[\hat{a}_j(t_0)\,{\rm e}^{-{\rm i}\omega_j(t-t_0)} + \hat{a}_j^\dagger(t_0)\,{\rm e}^{{\rm i}\omega_j(t-t_0)}\Big]. \tag{VI.110b}$$

This operator corresponds to a Langevin force, which only depends on freely evolving operators of the bath.[89] In turn, the first term on the right-hand side of Eq. (VI.110a) describes a retarded friction force exerted on the heavy particle by the bath, and due to the perturbation of the latter by the former at earlier times.

Limiting case of a continuous bath

Introducing as in Sec. V.3.3 c the *spectral density of the coupling to the bath*

$$J(\omega) \equiv \frac{\pi}{2} \sum_j \frac{C_j^2}{m_j\omega_j}\,\delta(\omega-\omega_j), \tag{VI.111}$$

and its continuous approximation $J_c(\omega)$ [cf. Eq. (V.75)] the retarded force in Eq. (VI.110a) becomes

$$\begin{aligned}\sum_{j=1}^{N} \frac{C_j^2}{2m_j\omega_j}\bigg[{\rm i}\int_{t_0}^{t} \hat{x}(t')\,{\rm e}^{-{\rm i}\omega_j(t-t')}\,{\rm d}t' + {\rm h.c.}\bigg] &= \frac{1}{\pi}\int J(\omega)\bigg[{\rm i}\int_{t_0}^{t} \hat{x}(t')\,{\rm e}^{-{\rm i}\omega(t-t')}\,{\rm d}t' + {\rm h.c.}\bigg]{\rm d}\omega \\ &\simeq \frac{1}{\pi}\int J_c(\omega)\bigg[{\rm i}\int_{t_0}^{t} \hat{x}(t')\,{\rm e}^{-{\rm i}\omega(t-t')}\,{\rm d}t' + {\rm h.c.}\bigg]{\rm d}\omega, \end{aligned} \tag{VI.112}$$

while the third term in that same equation can be rewritten as

$$-\Bigg(\sum_{j=1}^{N}\frac{C_j^2}{m_j\omega_j^2}\Bigg)\hat{x}(t) = -\bigg(\frac{2}{\pi}\int\frac{J(\omega)}{\omega}\,{\rm d}\omega\bigg)\hat{x}(t) \simeq -\bigg(\frac{2}{\pi}\int\frac{J_c(\omega)}{\omega}\,{\rm d}\omega\bigg)\hat{x}(t). \tag{VI.113}$$

With a trivial change of integration variable from t' to $\tau = t-t'$ and some rewriting, the retarded force (VI.112) becomes after exchanging the order of integrations

$$\frac{1}{\pi}\int\frac{J_c(\omega)}{\omega}\bigg[{\rm i}\omega\int_0^{t-t_0}\hat{x}(t-\tau)\,{\rm e}^{-{\rm i}\omega\tau}\,{\rm d}t' + {\rm h.c.}\bigg]{\rm d}\omega = -\frac{1}{\pi}\int_0^{t-t_0}\hat{x}(t-\tau)\,\frac{\rm d}{{\rm d}\tau}\bigg[\int\frac{J_c(\omega)}{\omega}\big({\rm e}^{-{\rm i}\omega\tau}+{\rm e}^{{\rm i}\omega\tau}\big)\,{\rm d}\omega\bigg]{\rm d}\tau.$$

Introducing the “memory kernel” [cf. Eq. (V.74)]

$$\gamma(\tau) \equiv \frac{2}{\pi}\int\frac{J_c(\omega)}{M\omega}\cos\omega\tau\,{\rm d}\omega \tag{VI.114}$$

and performing an integration by parts, in which the equation of motion (VI.108a) allows us to replace the time derivative of $\hat{x}(t)$ by $\hat{p}(t)/M$, the friction force becomes

$$-M\int_0^{t-t_0}\hat{x}(t-\tau)\,\gamma'(\tau)\,{\rm d}\tau = M\Big[\gamma(0)\hat{x}(t) - \gamma(t-t_0)\hat{x}(t_0)\Big] - \int_0^{t-t_0}\hat{p}(t-\tau)\,\gamma(\tau)\,{\rm d}\tau.$$

In many simple cases, corresponding to oscillator baths with a “short memory”, the kernel $\gamma(\tau)$ only takes significant values in a limit range of size ω_c^{-1} around $\tau = 0$. As soon as $|t-t_0| \gg \omega_c^{-1}$, the term $\gamma(t-t_0)$ in the above equation then becomes negligible, while the upper limit of the integral can be sent to $+\infty$ without affecting the result significantly. Deducing $\gamma(0)$ from Eq. (VI.114), the friction force (VI.112) reads

$$\frac{1}{\pi}\int J_c(\omega)\bigg[{\rm i}\int_{t_0}^{t}\hat{x}(t')\,{\rm e}^{-{\rm i}\omega(t-t')}\,{\rm d}t' + {\rm h.c.}\bigg]{\rm d}\omega = \bigg(\frac{2}{\pi}\int\frac{J_c(\omega)}{\omega}\,{\rm d}\omega\bigg)\hat{x}(t) - \int_0^{\infty}\hat{p}(t-\tau)\,\gamma(\tau)\,{\rm d}\tau.$$

The first term on the right hand side is exactly the negative of Eq. (VI.113): putting everything together, the evolution equation (VI.110a) takes the simple form of a generalized Langevin equation

$$\frac{{\rm d}\hat{p}(t)}{{\rm d}t} = -\int_0^{\infty}\hat{p}(t-\tau)\,\gamma(\tau)\,{\rm d}\tau + \hat{F}_{\rm L}(t). \tag{VI.115}$$

Dividing this equation by M, one obtains a similar evolution equation for the velocity operator $\hat{v}(t)$.

[89] One easily checks in a basis of energy eigenstates $\langle\hat{a}_j(t_0)\rangle_{\rm eq.} = \langle\hat{a}_j^\dagger(t_0)\rangle_{\rm eq.} = 0$ for all bath oscillators, which results in $\langle\hat{F}_{\rm L}(t)\rangle_{\rm eq.} = 0$.

Generalized susceptibility

Let us add to the Hamiltonian (VI.107) a perturbation $\hat{W} = -F_{\text{ext.}}(t)\hat{x}(t)$ coupling to the position of the Brownian particle. One easily checks that this perturbation amounts to adding an extra term $F_{\text{ext.}}(t)\hat{\mathbb{1}}$ on the right-hand side of Eq. (VI.115). Dividing the resulting equation by M, taking the average, and Fourier transforming, one obtains the generalized susceptibility [cf. Eq. (V.62)]

$$\tilde{\chi}_{vx}(\omega) = \frac{1}{M}\frac{1}{\tilde{\gamma}(\omega) - \mathrm{i}\omega}, \tag{VI.116a}$$

where $\tilde{\gamma}(\omega)$ is given by

$$\tilde{\gamma}(\omega) = \int \gamma(t)\,\Theta(t)\,\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t. \tag{VI.116b}$$

The Caldeira–Leggett Hamiltonian (VI.107) is invariant under time reversal. As already seen in § (VI.4.3 b), this leads to the proportionality between the spectral function $\tilde{\xi}_{vx}(\omega)$ and the real part of the generalized susceptibility $\tilde{\chi}_{vx}(\omega)$:

$$\tilde{\xi}_{vx}(\omega) = -\frac{\mathrm{i}}{M}\frac{\operatorname{Re}\tilde{\gamma}(\omega)}{|\tilde{\gamma}(\omega) - \mathrm{i}\omega|^2}.$$

If $\tilde{\gamma}(\omega)$ decreases quickly enough as $|\omega|$ goes to ∞—which depends on the specific behavior of $J_c(\omega)$ at infinity, see Eq. (VI.114)—, the spectral function $\tilde{\xi}_{vx}(\omega)$ can have moments to all orders, which can then obey the sum rules (VI.81).