Microscopic Origin of Dissipation

1 Introduction

One can read in textbooks on classical mechanics that *dissipation* that is usually taken into account by adding "phenomenological" *damping* terms in the equations of motion such as

$$m\ddot{\mathbf{r}} + 2m\gamma\dot{\mathbf{r}} + \frac{\partial U}{\partial \mathbf{r}} = 0$$

is itself of a non-mechanical origin because it is caused by the coupling of the system to the environment that is described statistically by temperature and other thermodynamic parameters. The origin of these statements goes back to the years when it was impossible to solve equations of motion for systems with a macroscopic number of degrees of freedom. However, with the growth of computing power solving equations of motion for large systems has become a matter of fact, and a new area of physics, computer simulations, has emerged. Of course, simulating real macroscopic systems with an Avogadro number $N_A \sim 10^{23}$ particles is still prohibitive. Nevertheless, it turns out that using only $N \sim 10^3 - 10^5$ particles is sufficient to describe macroscopic properties of many systems.

Already in the IX century Ludwig Boltzmann and other researchers argued about apparent irreversibility and dissipation in conservative many-body systems that obey deterministic equations of motion. Boltzmann himself obtained his famous kinetic equation under the assumption of the "molecular chaos" that introduced irreversibility "by hand". Some physicists desagreed with this saying that the true equations are reversible and after making the Poincaré cycle the system will return into the initial state, that is a rigorous mathematical result. Practically, however, for macroscopic systems the Poincaré cycle (the recurrence time) is longer than the age of the Universe, so that a gas initially held in one half of the container will never completely return into this half after the separating wall is removed.

Still, some of the XX-century physicists believed that going beyond the deterministic mechanics is needed to describe irreversibility and dissipation. However, computer simulations on conservative mechanical systems show that the recurrence phenomena, still visible for moderate-size systems, quickly disappear as the size is increased, so that practically irreversible relaxation is observed. This means that dissipation is in fact a mechanical phenomenon.

2 The model

In addition to computer simulations, it was found that for some models irreversibility can be described analytically. One of these models is a model of an oscillator weakly coupled to many harmonic oscillators with widely distributed frequencies:

$$\mathcal{L} = \frac{m_0}{2}\left(\dot{X}^2 - \omega_0^2 X^2\right) + \sum_{i=1}^{N}\frac{m_i}{2}\left(\dot{x}_i^2 - \omega_i^2 x_i^2\right) - X\sum_{i=1}^{N}C_i x_i. \tag{1}$$

The last term of this expression is the linear (more precisely, bilinear) coupling of the "central" oscillator x to the "environment" or "bath" of many oscillators x_i . The equations of motion for this model have the form

$$
\begin{aligned}
m_0\left(\ddot{X} + \omega_0^2 X\right) + \sum_{i=1}^{N}C_i x_i &= 0 \\
m_i\left(\ddot{x}_i + \omega_i^2 x_i\right) + C_i X &= 0.
\end{aligned}
\tag{2}
$$

Searching for the solution in the form

$$X(t) = a \cos (\Omega t - \Phi), \qquad x_i(t) = a_i \cos (\Omega t - \varphi_i) \tag{3}$$

one obtains the system of linear equations

$$
\begin{aligned}
m_0 \left(-\Omega^2 + \omega_0^2\right) a + \sum_{i=1}^{N} C_i a_i &= 0 \\
m_i \left(-\Omega^2 + \omega_i^2\right) a_i + C_i a &= 0, \qquad i = 1 \ldots N
\end{aligned}
\tag{4}
$$

that defines the eigenfrequencies and normal modes of the system. It is easy to obtain the secular equation. Expressing a_i through a using the second line, inserting the result into the first equation, and dividing the result by a one obtains

$$\Omega^2 - \omega_0^2 - \sum_{i=1}^{N} \frac{C_i^2}{m_0 m_i \left(\Omega^2 - \omega_i^2\right)} = 0. \tag{5}$$

3   Analytical solution

This is, in fact, a $(N+1)$th order algebraic equation for Ω^2 and it can be solved numerically, as well as the whole eigenvalue problem of Eq. (4). However, in the case of weak coupling C_i one can find the correction to the frequency of the central oscillator perturbatively. Denoting this perturbed frequency $\Omega \Rightarrow \tilde{\omega}_0$, and replacing $\Omega \to \omega_0$ in the denominator, for the latter one obtains

$$\tilde{\omega}_0^2 \cong \omega_0^2 - \frac{1}{m_0} \sum_{i=1}^{N} \frac{C_i^2}{m_i \left(\omega_i^2 - \omega_0^2\right)}. \tag{6}$$

Of course, this exression makes sense only if ω_0 is not too close to one of the frequencies ω_i, otherwise this perturbation theory becomes invalid. This condition, however, becomes irrelevant if the number of the bath oscillators tends to infinity so that one can replace summation by integration. The latter is a crucial step that introduces irreversibility on the analytical level. With the function

$$\lambda(\omega) = \sum_{i=1}^{N} \frac{C_i^2}{m_i} \delta \left(\omega - \omega_i\right) \tag{7}$$

that is related to the density of bath states

$$\rho(\omega) = \frac{1}{N} \sum_{i=1}^{N} \delta \left(\omega - \omega_i\right) \tag{8}$$

one can rewrite Eq. (6) as

$$\tilde{\omega}_0^2 \cong \omega_0^2 - \frac{1}{m_0} \int_0^\infty \frac{d\omega \lambda(\omega)}{\omega^2 - \omega_0^2}. \tag{9}$$

One can easily see that this expression is still equivalent to Eq. (6) since one can step back from Eq. (9) to Eq. (6) using Eq. (7). The really crucial step is to consider now $\lambda(\omega)$ as a *continuous* function of ω rather than as a collection of δ-functions. Then Eq. (9) becomes a *true* integral that depends on how the singularity at $\omega = \omega_0$ is treated. Interpreting the intergal in Eq. (9) as a principal-value integral

$$\int_0^\infty \frac{d\omega \lambda(\omega)}{\omega^2 - \omega_0^2} \to \text{V.P.} \int_0^\infty \frac{d\omega \lambda(\omega)}{\omega^2 - \omega_0^2} = \lim_{\varepsilon \to 0} \left(\int_0^{\omega_0 - \varepsilon} \frac{d\omega \lambda(\omega)}{\omega^2 - \omega_0^2} + \int_{\omega_0 + \varepsilon}^\infty \frac{d\omega \lambda(\omega)}{\omega^2 - \omega_0^2} \right)$$

(V.P. = Valeur Principal) gives a small real correction to ω_0 that is not interesting. A striking feature of the integral in Eq. (9) is, however, that it is unstable with respect to adding a vanishingly small imaginary

2

constant to ω, that is, $\omega \rightarrow \omega + i\delta$ with $\delta \rightarrow 0$. Doing this is equivalent to shifting the integration contour up or down from the real axis into the complex plane that results in avoiding the singularity. With $i\delta$ added, Eq. (9) takes the form

$$\tilde{\omega}_0^2 = \omega_0^2 - \frac{1}{m_0} \int_0^\infty \frac{d\omega \lambda(\omega)}{(\omega + i\delta)^2 - \omega_0^2} = \omega_0^2 - \frac{1}{m_0} \int_0^\infty \frac{d\omega \lambda(\omega)}{(\omega + \omega_0)(\omega - \omega_0 + i\delta)}.$$

Note that we kept $i\delta$ only in the singular factor with $\omega - \omega_0$, in all other places $i\delta$ is irrelevant. Then using the formula

$$\frac{1}{x \pm i0} = \frac{1}{x} \mp i\pi\delta(x)$$

(the second term stemming from making a half-circle around the pole at $\omega = \omega_0$ in the complex plane) one obtains

$$\tilde{\omega}_0^2 = \omega_0^2 - \frac{1}{m_0}\text{V.P.} \int_0^\infty \frac{d\omega \lambda(\omega)}{\omega^2 - \omega_0^2} + \frac{i\pi\lambda(\omega_0)}{2m_0\omega_0} \Rightarrow \omega_0^2 + \frac{i\pi\lambda(\omega_0)}{2m_0\omega_0}\text{sign}(\delta), \tag{10}$$

where we have dropped the small real correction to the frequency and $\text{sign}(\delta)$ is defined as

$$\text{sign}(\delta) = \begin{cases} -1, & \delta < 0 \\ 0, & \delta = 0 \\ 1 & \delta > 0. \end{cases}$$

The imaginary term in Eq. (10) cannot simply be ignored as it does not vanish in the limit $\delta \rightarrow 0$. But this term requires interpretation. What does a complex frequency mean? To clarify this, one can rewrite Eq. (3) as

$$X(t) = a \, \text{Re} \, e^{i(\tilde{\Omega}t - \Phi)}, \qquad x_i(t) = a_i \, \text{Re} \, e^{i(\tilde{\Omega}t - \varphi_i)}. \tag{11}$$

For a complex $\tilde{\Omega}$ in the form

$$\tilde{\Omega} = \Omega + i\Gamma$$

one obtains

$$X(t) = ae^{-\Gamma t} \cos(\Omega t - \Phi), \qquad x_i(t) = a_i e^{-\Gamma t} \cos(\Omega t - \varphi_i)$$

that describes damped oscillations. Thus, with the convention of Eq. (11), the imaginary part of Ω should be positive, to avoid physically inacceptable exponentially growing solution. Now it becomes clear that formal replacing $\omega \rightarrow \omega + i\delta$ with $\delta \rightarrow +0$ in Eq. (9) can be interpreted as taking into account a *vanishingly small* damping of the bath oscillators. This does not contradict anything since, as just said, the damping of bath oscillators tends to zero and we do not change the initial model. On the other hand, taking $\delta < 0$ for the bath oscillators would be physically inacceptable since this would result in a solution slowly diverging at large times. The vanishingly small damping of the bath oscillators makes, however, a big effect on the central oscillator that acquires a *finite* damping because of the coupling to the environment. From Eq. (10) with $\delta > 0$ one obtains

$$\tilde{\omega}_0 = \sqrt{\omega_0^2 + \frac{i\pi\lambda(\omega_0)}{2m_0\omega_0}} \cong \omega_0 + i\Gamma_0,$$

where the damping Γ_0 is given by

$$\Gamma_0 = \frac{\pi\lambda(\omega_0)}{4m_0\omega_0^2} = \frac{\pi}{4\omega_0^2} \sum_{i=1}^N \frac{C_i^2}{m_0 m_i} \delta(\omega - \omega_i). \tag{12}$$

Now one can forget about the bath oscillators and just use the damped equation of motion

$$\ddot{X} + 2\Gamma_0 \dot{X} + \omega_0^2 X = 0 \tag{13}$$

for the central oscillator. Searching for the solution in the form

$$X(t) \sim \mathrm{Re}\, e^{i\tilde{\Omega}t}$$

one obtains the secular equation

$$-\tilde{\Omega}^2 + 2i\Gamma_0\tilde{\Omega} + \omega_0^2 = 0.$$

For small damping $\Gamma_0 \ll \omega_0$ the complex eigenfrequency is approximately

$$\tilde{\Omega} = \sqrt{\omega_0^2 + 2i\Gamma_0\tilde{\Omega}} \cong \sqrt{\omega_0^2 + 2i\Gamma_0\omega_0} \cong \omega_0 + i\Gamma_0.$$

The final solution taking into account the initial conditions at $t = 0$ has the form

$$X(t) = \left[X(0)\cos(\omega_0 t) + \dot{X}(0)\frac{\sin(\omega_0 t)}{\omega_0} \right] e^{-\Gamma_0 t}. \tag{14}$$

The energy of the central oscillator is given by

$$E(t) = \frac{m}{2}\left[\dot{X}^2(t) + \omega_0^2 X^2(t) \right] = E(0)e^{-2\Gamma_0 t}, \tag{15}$$

where

$$E(0) = \frac{m}{2}\left[\dot{X}^2(0) + \omega_0^2 X^2(0) \right]$$

and we haven't differentiated the slow function $e^{-\Gamma_0 t}$.

The results obtained explain that Eq. (13) that is sometimes interpreted as a "phenomenological" equation with a non-mechanical damping term $2\Gamma_0\dot{X}$ added by hand can be in fact obtained from a purely mechanical and conservative model.

4   Numerical solution

To produce a numerical solution of the problem, one can write Eq. (2) in the vectorized form

$$\mathbf{M} \cdot \ddot{\mathbf{X}} + \mathbf{K} \cdot \mathbf{X} = \mathbf{0}. \tag{16}$$

where $\mathbf{X}$ is the original-coordinate vector, $\mathbf{X} = (X, x_1, x_2, \ldots x_N)$, $\mathbf{M}$ is a diagonal matrix and $\mathbf{K}$ contains diagonal and nondiagonal terms:

$$
\begin{aligned}
M_{ij} &= m_i \delta_{ij}, & i &= 0, 1, \ldots, N \\
K_{ii} &= m_i \omega_i^2, & i &= 0, 1, \ldots, N \\
K_{0i} &= K_{i0} = C_i, & i &= 1, \ldots, N.
\end{aligned}
$$

The eigenvalue problem, Eq. (4), reads

$$\left(-\Omega^2 \mathbf{M} + \mathbf{K} \right) \cdot \mathbf{a} = \mathbf{0}. \tag{17}$$

There are $N+1$ eigenvalues Ω_α^2 and eigenvectors $\mathbf{a}_\alpha$, $\alpha = 0, 1, \ldots, N$ that satisfy the orthogonality condition

$$\mathbf{a}_\alpha^T \cdot \mathbf{M} \cdot \mathbf{a}_\beta = \delta_{\alpha\beta}$$

($\mathbf{a}_\beta$ are columns and $\mathbf{a}_\alpha^T$ are rows). One can stack all $\mathbf{a}_\alpha$ into the $(N+1) \times (N+1)$ matrix $\mathbf{A}$ that is orthogonal with respect to $\mathbf{M}$:

$$\mathbf{A}^T \cdot \mathbf{M} \cdot \mathbf{A} = \mathbf{I}, \tag{18}$$

where $\mathbf{I}$ is a unit matrix, $I_{\alpha\beta} = \delta_{\alpha\beta}$. From Eq. (17) follows

$$\mathbf{a}_\alpha^T \cdot \mathbf{K} \cdot \mathbf{a}_\beta = \Omega_\alpha^2 \delta_{\alpha\beta}, \qquad \mathbf{A}^T \cdot \mathbf{K} \cdot \mathbf{A} = \mathbf{\Omega}^2 \equiv \mathrm{diag}\left(\Omega_\alpha^2\right). \tag{19}$$

Further one can introduce the normal-coordinate vector $\boldsymbol{\zeta}$ by

$$\mathbf{X} = \mathbf{A} \cdot \boldsymbol{\zeta}, \qquad \mathbf{X}^T = (\mathbf{A} \cdot \boldsymbol{\zeta})^T = \boldsymbol{\zeta}^T \cdot \mathbf{A}^T. \tag{20}$$

These equations can be resolved for $\boldsymbol{\zeta}$ and ζ_α:

$$\boldsymbol{\zeta} = \mathbf{A}^{-1} \cdot \mathbf{X}, \qquad \zeta_\alpha = \sum_{i=0}^{N} \left(\mathbf{A}^{-1}\right)_{\alpha i} x_i. \tag{21}$$

Inserting $\mathbf{X} = \mathbf{A} \cdot \boldsymbol{\zeta}$ into Eq. (16), multiplying by $\mathbf{A}^T$ from left, and using Eqs. (18) and (19), one obtains the equation of motion for the normal coordinates in the simple form

$$\ddot{\boldsymbol{\zeta}} + \mathbf{\Omega}^2 \cdot \boldsymbol{\zeta} = \mathbf{0}$$

or

$$\ddot{\zeta}_\alpha + \Omega_\alpha^2 \zeta_\alpha = 0, \qquad \alpha = 0, 1, \ldots, N.$$

The solution of these equations is

$$\begin{aligned}
\zeta_\alpha(t) &= \zeta_\alpha(0) \cos\left(\Omega_\alpha t\right) + \dot{\zeta}_\alpha(0) \frac{\sin\left(\Omega_\alpha t\right)}{\Omega_\alpha} \\
&= \sum_{i=0}^{N} \left(\mathbf{A}^{-1}\right)_{\alpha i} \left[x_i(0) \cos\left(\Omega_\alpha t\right) + \dot{x}_i(0) \frac{\sin\left(\Omega_\alpha t\right)}{\Omega_\alpha}\right].
\end{aligned}$$

This resut also can be brought in a vectorized form (excercize). Finally, from Eq. (20) one obtains

$$x_i(t) = \sum_{\alpha=0}^{N} a_{i\alpha} \zeta_\alpha(t) = \sum_{\alpha=0}^{N} \sum_{j=0}^{N} a_{i\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha j} \left[x_i(0) \cos\left(\Omega_\alpha t\right) + \dot{x}_i(0) \frac{\sin\left(\Omega_\alpha t\right)}{\Omega_\alpha}\right].$$

In particular, if in the initial state only the central oscillator $X \equiv x_0$ was in a general state, whereas the bath oscillators were in their ground states, for the central oscillator one obtains

$$X(t) = \sum_{\alpha=0}^{N} a_{0\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 0} \left[X(0) \cos\left(\Omega_\alpha t\right) + \dot{X}(0) \frac{\sin\left(\Omega_\alpha t\right)}{\Omega_\alpha}\right].$$

Let us now calculate the energy of the central oscillator. Using

$$\dot{X}(t) = \sum_{\alpha=0}^{N} a_{0\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 0} \left[-X(0)\Omega_\alpha \sin\left(\Omega_\alpha t\right) + \dot{X}(0) \cos\left(\Omega_\alpha t\right)\right]$$

one obtains

$$\begin{aligned}
E(t) &= \frac{m}{2} \left[\dot{X}^2(t) + \omega_0^2 X^2(t)\right] = \frac{m}{2} \sum_{\alpha,\beta=0}^{N} a_{0\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 0} a_{0\beta} \left(\mathbf{A}^{-1}\right)_{\beta 0} \\
&\quad \times \left\{\left[-X(0)\Omega_\alpha \sin\left(\Omega_\alpha t\right) + \dot{X}(0) \cos\left(\Omega_\alpha t\right)\right]\left[-X(0)\Omega_\beta \sin\left(\Omega_\beta t\right) + \dot{X}(0) \cos\left(\Omega_\beta t\right)\right] \right. \\
&\quad \left. + \omega_0^2 \left[X(0) \cos\left(\Omega_\alpha t\right) + \dot{X}(0) \frac{\sin\left(\Omega_\alpha t\right)}{\Omega_\alpha}\right]\left[X(0) \cos\left(\Omega_\beta t\right) + \dot{X}(0) \frac{\sin\left(\Omega_\beta t\right)}{\Omega_\beta}\right]\right\}
\end{aligned}$$

5

$$
= \frac{m}{2} \sum_{\alpha,\beta=0}^{N} a_{0\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 0} a_{0\beta} \left(\mathbf{A}^{-1}\right)_{\beta 0}
$$

$$
\times \left\{ X^2(0) \left[\Omega_\alpha \Omega_\beta \sin\left(\Omega_\alpha t\right) \sin\left(\Omega_\beta t\right) + \omega_0^2 \cos\left(\Omega_\alpha t\right) \cos\left(\Omega_\beta t\right) \right] \right.
$$

$$
+ \dot{X}^2(0) \left[\cos\left(\Omega_\alpha t\right) \cos\left(\Omega_\beta t\right) + \frac{\omega_0^2}{\Omega_\alpha \Omega_\beta} \sin\left(\Omega_\alpha t\right) \sin\left(\Omega_\beta t\right) \right]
$$

$$
\left. + X(0)\dot{X}(0) \left[\sin\left(\Omega_\alpha t\right) \cos\left(\Omega_\beta t\right) \left(-\Omega_\alpha + \frac{\omega_0^2}{\Omega_\alpha} \right) + (\alpha \rightleftharpoons \beta) \right] \right\}. \tag{22}
$$

Analytically this expression has nothing in common with Eq. (15) that shows a slow relaxation of the energy. Still, for N sufficiently large both expression numerically coincide. In Eq. (22), decreasing of $E(t)$ is due to many sinusoidal functions with different frequencies that go out of phase and interfere destructively with increasing time.

Numerical simulations can be done, for instance, with the equidistant spectrum of bath oscillators

$$
\omega_i = \omega_{\min} + \frac{i-1}{N-1}\omega_{\max}, \qquad \omega_{\min} < \omega_0 < \omega_{\max},
$$

so that $\omega_1 = \omega_{\min}$ and $\omega_N = \omega_{\max}$, and one can set all C_i and m_i equal to each other:

$$
C_i = \frac{C}{\sqrt{N}}, \qquad m_0 = m_i = m = 1.
$$

With this choice the matrix $\mathbf{M}$ becomes a unit matrix, thus from Eq. (18) follows $\mathbf{A}^{-1} = \mathbf{A}^T$ and thus $\left(\mathbf{A}^{-1}\right)_{\alpha 0} = a_{0\alpha}$. If, on addition, $\dot{X}(0) = 0$, then Eq. (22) simplifies to

$$
\frac{E(t)}{E(0)} = \sum_{\alpha,\beta=0}^{N} (a_{0\alpha}a_{0\beta})^2 \left[\cos\left(\Omega_\alpha t\right)\cos\left(\Omega_\beta t\right) + \frac{\Omega_\alpha \Omega_\beta}{\omega_0^2} \sin\left(\Omega_\alpha t\right)\sin\left(\Omega_\beta t\right) \right]
$$

$$
= \left[\sum_{\alpha=0}^{N} a_{0\alpha}^2 \cos\left(\Omega_\alpha t\right) \right]^2 + \frac{1}{\omega_0^2} \left[\sum_{\alpha=0}^{N} a_{0\alpha}^2 \Omega_\alpha \sin\left(\Omega_\alpha t\right) \right]^2. \tag{23}
$$

Note that the second form of this expression requires only $\sim N$ operations to perform and is much faster to compute. It is not difficult to program Eq. (23) in Wolfram Mathematica.

On the other hand, Eq. (12) becomes

$$
\Gamma_0 = \frac{\pi\lambda(\omega_0)}{4m_0\omega_0^2} = \frac{\pi}{4\omega_0^2}\frac{C^2}{m^2}\frac{1}{N}\sum_{i=1}^{N}\delta\left(\omega_0 - \omega_i\right) = \frac{\pi}{4\omega_0^2}\frac{C^2}{m^2}\rho(\omega_0).
$$

Since for this model the density of states of the bath oscillators is

$$
\rho(\omega) = \frac{1}{\omega_{\max} - \omega_{\min}}
$$

(so that their total number is $N = N\int_{\omega_{\min}}^{\omega_{\max}} d\omega\rho(\omega) = N$), from Eq. (15) one finally obtains

$$
\frac{E(t)}{E(0)} = \exp\left(-2\Gamma_0 t\right) = \exp\left[-\frac{\pi}{2}\left(\frac{C}{m\omega_0}\right)^2 \frac{t}{\omega_{\max} - \omega_{\min}} \right] \tag{24}
$$

with $m = 1$. Eqs. (23) and (24) are numerically compared with each other in the figure below for different values of N. One can see that there is a recurrence phenomenon for finite N but as N grows the recurrence time becomes longer, so that the recurrence goes out of the window. For times smaller than the recurrence time, there is a very good agreement between the analytical and numerical results.