Linear Response

Suppose we have an equilibrium macroscopic system (no matter, quantum or classical) and a weak time-dependent perturbation of the form

$$V(t) \;=\; -xf(t) \;, \tag{1}$$

where V is the perturbation potential energy, x is one of generalized coordinates of the system, and f is a time-dependent generalized force. If $V \equiv 0$, then the system is in equilibrium and $\bar{x}(t) \equiv 0$, where $\bar{x}$ is the coordinate x averaged over corresponding equilibrium ensemble of states. The question now is what is the generic form of $\bar{x}(t)$, provided $f(t) \neq 0$, but arbitrarily small. The smallness of $|f|$ implies the linearity of the response as a functional of f. The causality requires that the response at time t comes from times $t_1 \leq t$. The most general form of a functional satisfying the linearity and causality constraints is

$$\bar{x}(t) \;=\; \int_{-\infty}^{t} \alpha(t,t_1) f(t_1)\, dt_1 \;, \tag{2}$$

where α is some f-independent function. Finally, the time-translation invariance (independence of the unperturbed Hamiltonian on time) requires

$$\alpha(t,t_1) \;\equiv\; \alpha(t-t_1) \;, \tag{3}$$

and thus

$$\bar{x}(t) \;=\; \int_{-\infty}^{t} \alpha(t-t_1) f(t_1)\, dt_1 \;\equiv\; \int_0^{\infty} \alpha(\tau) f(t-\tau)\, d\tau \;. \tag{4}$$

Hence, the response of the system to a weak force f is totally described by a function $\alpha(\tau)$ defined in the region $\tau \geq 0$. In what follows, we confine ourselves with the case when the static response—time-independent f—is well defined. This implies convergence of the integral

$$\int_0^{\infty} \alpha(\tau)\, d\tau \;. \tag{5}$$

Now comes a very practical question: What is the easiest way to measure $\alpha(\tau)$ experimentally? It is amazing that to answer this most practical question a deep theoretical complex-number analysis is crucial. To this end, consider a response of the system to a harmonic perturbation

$$f(t) \;=\; f_0 \cos(\omega t) \;\equiv\; (f_0/2)\left[\mathrm{e}^{i\omega t} + \mathrm{e}^{-i\omega t} \right] \;. \tag{6}$$

The representation of cosine in terms of two complex exponentials is very helpful since after plugging it into (4) the variables t and τ factorize, and we get

$$\bar{x}(t) \;=\; (f_0/2)\left[\alpha_\omega^* \mathrm{e}^{i\omega t} + \alpha_\omega \mathrm{e}^{-i\omega t}\right] \;\equiv\; f_0 |\alpha_\omega| \cos(\omega t - \varphi_\omega) \;, \tag{7}$$

where

$$\alpha_\omega \;=\; \int_0^\infty \alpha(\tau)\, \mathrm{e}^{i\omega\tau}\, d\tau \;, \tag{8}$$

which implies—because $\alpha(\tau)$ is real—

$$\alpha_{-\omega} \;=\; \alpha_\omega^* \;. \tag{9}$$

The phase shift φ_ω comes from the phase of α_ω:

$$\alpha_\omega \;\equiv\; |\alpha_\omega|\, \mathrm{e}^{i\varphi_\omega} \;. \tag{10}$$

From (7) we see that (i) the response is harmonic and (ii) by measuring the amplitude and *phase shift* of the response we get α_ω by Eq. (10). The theory of Fourier transforms—we will cover it later on in this course—says that if α_ω is defined by (8) then it contains a complete information about $\alpha(\tau)$ at $\tau \geq 0$, and, moreover, the latter can be restored by doing the integral

$$\alpha(\tau) \;=\; \int_{-\infty}^{\infty} \alpha_\omega\, \mathrm{e}^{-i\omega\tau}\, d\omega/2\pi \;. \tag{11}$$

Hence, by measuring the amplitude and phase shift of a harmonic response for all frequencies we can find $\alpha(\tau)$.

It turns out, however, that we can do an easier job by measuring just the *energy absorption rate* as a function of frequency of harmonic perturbation. This surprising fact relies on the Kramers-Kronig dispersion relations.

Consider the (averaged over a period of oscillation $2\pi/\omega$) amount of energy absorbed by the system per unit time, which is known to be given by the following formula

$$\Omega \;=\; -(\omega/2\pi) \int_0^{2\pi/\omega} \bar{x}(t)\, \dot{f}(t)\, dt \;. \tag{12}$$

In Quantum Mechanics, this relation is derived as follows.

$$\frac{dE}{dt} \;=\; \frac{d}{dt}\,\langle\psi(t)|H(t)|\psi(t)\rangle \;=\; \left\langle\dot{\psi}|H|\psi\right\rangle + \left\langle\psi|\dot{H}|\psi\right\rangle + \left\langle\psi|H|\dot{\psi}\right\rangle$$
$$=\; i\left\langle\dot{\psi}|\dot{\psi}\right\rangle + \left\langle\psi|\dot{H}|\psi\right\rangle - i\left\langle\dot{\psi}|\dot{\psi}\right\rangle \;=\; \left\langle\psi|\dot{H}|\psi\right\rangle \;=\; -\dot{f}\,\langle\psi|x|\psi\rangle \;\equiv\; -\dot{f}\bar{x} \;. \tag{13}$$

Here H is the total Hamiltonian of the system, including the perturbation; its time dependence is totally due to $f(t)$. Then we just need to average this expression over a period of oscillation.

We have

$$\Omega \ = \ -(f_0^2\omega/8\pi)\int_0^{2\pi/\omega}\left[\alpha_\omega^* \mathrm{e}^{i\omega t}+\alpha_\omega \mathrm{e}^{-i\omega t}\right]\left[i\omega \mathrm{e}^{i\omega t}-i\omega \mathrm{e}^{-i\omega t}\right]dt\ . \qquad (14)$$

Doing the integral kills the oscillating terms and we end up with the very important result

$$\Omega \ = \ (f_0^2\omega/2)\,\mathrm{Im}\,\alpha_\omega\ . \qquad (15)$$

The energy absorption rate is quadratic in the amplitude of perturbation and is proportional to the imaginary part of α_ω. That is to find $\mathrm{Im}\,\alpha_\omega$ we just need to measure Ω:

$$\mathrm{Im}\,\alpha_\omega \ = \ \frac{2\Omega}{f_0^2\,\omega}\ . \qquad (16)$$

The real part of α can be found then by Kramers-Kronig relation. Indeed, the convergence of the integral (5) guaranties the convergence of the integral (8) for any complex ω, provided $\mathrm{Im}\,\omega \geq 0$. Hence, α_ω has no singularities in the upper half-plane of complex ω, including the real axis. This justifies the applicability of the dispersion relations.

Introducing short-hand notation

$$\alpha'_\omega \ = \ \mathrm{Re}\,\alpha_\omega\ , \qquad \alpha''_\omega \ = \ \mathrm{Im}\,\alpha_\omega\ , \qquad (17)$$

we have

$$\alpha'_{\omega_0} \ = \ \frac{1}{\pi}\,\mathrm{P}\int_{-\infty}^{\infty}\frac{\alpha''_\omega}{\omega-\omega_0}\,d\omega\ . \qquad (18)$$

We can also exclude negative frequencies by noting that from (9) it follows that

$$\alpha'_{-\omega} \ = \ \alpha'_\omega\ , \qquad \alpha''_{-\omega} \ = \ -\alpha''_\omega\ , \qquad (19)$$

and thus

$$\alpha'_{\omega_0} \ = \ \frac{2}{\pi}\,\mathrm{P}\int_0^{\infty}\frac{\omega\alpha''_\omega}{\omega^2-\omega_0^2}\,d\omega\ . \qquad (20)$$

Summarizing, the procedure of experimentally obtaining the linear response function $\alpha(\tau)$ is as follows.

(i) Find α''_ω by measuring the energy absorption rate, Eq. (16).

(ii) Find α'_ω from Kramers-Kronig relation (20).

(iii) Find $\alpha(\tau)$ by doing the integral (11), which in view of (19) reduces to

$$\alpha(\tau) \ = \ (1/\pi)\int_0^{\infty}\left[\alpha'_\omega\cos\omega\tau \ + \ \alpha''_\omega\sin\omega\tau\right]d\omega\ . \qquad (21)$$