Linear response theory

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Linear response theory is a special instance of first order perturbation theory. Its purpose is to describe the response of a mechanical system to external forces in the regime of weak forcing. Of particular interest is the response of systems which are driven out of some dynamical equilibrium by non-conservative mechanical forces or thermal forces like temperature or density gradients. This article is a short introduction to some mathematical results in quantum mechanical linear response theory. We refer to [KTH] for an introduction to the physical aspects of the subject.

1 Finite time linear response

The first problem of linear response theory is the determination of the response of the system to the action of the driving forces over a finite interval of time. We shall consider separately the simple case of mechanical forcing and the more delicate thermal drives.

The unperturbed system is a C^*- or W^*-dynamical system $(\mathcal{O}, \tau)$ equipped with a modular invariant state ω. We denote by δ the generator of the dynamics τ, by σ the modular group of ω and by ζ its generator. $\mathcal{O}_{\rm self}$ further denotes the set of selfadjoint elements of $\mathcal{O}$. We note that the important role of the modular structure in linear response theory was already apparent in [NVW].

Since ω is $(\sigma, -1)$-KMS, for any $A, B \in \mathcal{O}$ there exists a function $F(A, B; z)$ which is analytic in the strip $\{z \,|\, -1 < \operatorname{Im} z < 0\}$, bounded and continuous on its closure and such that $F(A, B; \theta) = \omega(A\sigma^\theta(B))$ and $F(A, B; \theta - \mathrm{i}) = \omega(\sigma^\theta(B)A)$ for $\theta \in \mathbb{R}$. We shall abuse notation and denote $F(A, B; z)$ by either $\omega(A\sigma^z(B))$ or $\omega(\sigma^{-z}(A)B)$ for $-1 \le \operatorname{Im} z \le 0$. In particular, the canonical correlation of $A, B \in \mathcal{O}$ is defined by

$$\langle A|B\rangle_\omega = \int_0^1 \omega(A\sigma_\omega^{-\mathrm{i}\theta}(B))\,\mathrm{d}\theta = \int_0^1 F(A, B; -\mathrm{i}\theta)\,\mathrm{d}\theta.$$

One easily checks that it defines an inner product on the real vector space $\mathcal{O}_{\rm self}$ (see [NVW]).

1.1 Mechanical drive

Let $\tau_V^{s\to t}$ be the dynamics on $\mathcal{O}$ generated by $\delta + \mathrm{i}[V(t), \cdot\,]$, i.e., the solution of

$$\partial_t \tau_V^{s\to t}(A) = \tau_V^{s\to t}(\delta(A) + \mathrm{i}[V(t), A]), \quad \partial_s \tau_V^{s\to t}(A) = \delta(\tau_V^{s\to t}(A)) + \mathrm{i}[V(s), (\tau_V^{s\to t}(A)]),$$

which satisfies $\tau_V^{s\to t}(A) = A$ for $s = t$. For simplicity, we assume that $t \mapsto V(t)$ belongs to $C(\mathbb{R}, \mathcal{O}_{\rm self})$. Standard time-dependent perturbation theory yields (see [Quantum dynamical systems])

$$\tau_V^{s\to t}(A) = \tau^{t-s}(A) + \int_s^t \mathrm{i}[\tau^{u-s}(V(u)), \tau^{t-u}(A)]\,\mathrm{d}u + \text{higher order terms}.$$

Thus, to first order in the perturbation V, the change $\omega \circ \tau_V^{s\to t} - \omega$ is given by

$$(\Delta\omega)^{s\to t} = \int_s^t \mathcal{K}(t-u)V(u)\,\mathrm{d}u.$$

The operator valued response function $\mathcal{K}(u) : \mathcal{O} \to \mathcal{O}^{\#}$, where $\mathcal{O}^{\#}$ denotes the dual of $\mathcal{O}$, is defined by

$$(\mathcal{K}(u)V)(A) = \omega(\mathrm{i}[V, \tau^u(A)]), \tag{1}$$

for $u \geq 0$ and $\mathcal{K}(u) = 0$ for $u < 0$ (causality).

Note that if ω is mixing for $(\mathcal{O}, \tau)$ then $\lim_{t\to\infty}(\Delta\omega)^{s\to t}(X) = 0$ for any $V \in C(\mathbb{R}, \mathcal{O}_{\mathrm{self}})$ of compact support and any $X \in \mathcal{O}$, i.e., the system recovers from infinitesimal localized perturbations. We refer to [VW] for further connections between the mixing property and linear response theory.

For $V \in \mathrm{Dom}(\zeta)$, Equ. (1) can be rewritten as

$$(\mathcal{K}(u)V)(A) = \langle \tau^u(A) | \zeta(V) \rangle_\omega.$$

This is a typical fluctuation-dissipation relation: On the left hand side the response function $\mathcal{K}$ describes dissipation, the correlation function on the right hand side measures fluctuations.

For later reference let us consider the special case where ω is (τ, β)-KMS and $V(t) = -\sum_j X_j(t) A_j$. There the $A_j \in \mathcal{O}_{\mathrm{self}} \cap \mathrm{Dom}(\delta)$ describe the coupling of the system to external fields and the $X_j(t)$ are the time-dependent field strengths. One has $\zeta = -\beta\delta$ and the observable $\Phi_j = \delta(A_j)$ describes the flux conjugate to A_j. The linear response is given by the finite time Green-Kubo formula

$$(\Delta\omega)^{s\to t}(A) = \sum_j \beta \int_s^t \langle \tau^{t-u}(A) | \Phi_j \rangle_\omega \, X_j(u) \, \mathrm{d}u. \tag{2}$$

1.2 Thermal drive

To discuss thermal forcing we need more structure. We consider the setting of [NESS in quantum statistical mechanics]: A small system $\mathcal{S}$, described by $(\mathcal{O}_0, \tau_0)$ coupled to infinite reservoirs $\mathcal{R}_1, \ldots, \mathcal{R}_M$ described by $(\mathcal{O}_j, \tau_j)$, with $1 \leq j \leq M$. The algebra factorizes accordingly $\mathcal{O} = \otimes_{0\leq a\leq M} \mathcal{O}_a$ and the dynamics of the decoupled system is $\tau_{\mathrm{dec}} = \otimes_{0\leq a\leq M} \tau_a = \mathrm{e}^{t\delta_{\mathrm{dec}}}$. We denote by δ_a the generator of τ_a so that $\delta_{\mathrm{dec}} = \sum_a \delta_a$.

The dynamics τ of the coupled system is defined as the local perturbation of τ_{dec} by the coupling $V = \sum_{1\leq j\leq M} V_j$, where $V_j \in \mathcal{O}_0 \otimes \mathcal{O}_j$. Its generator is $\delta = \delta_{\mathrm{dec}} + \mathrm{i}[V, \cdot\,]$.

For simplicity we shall only consider here the case where the fiducial state ω is (τ, β)-KMS, so that the generator of its modular group is $\zeta = -\beta\delta$. We study small departures from this state resulting from imposed temperature gradients trough the system. Our discussion can easily be generalized to include other thermodynamic forces like inhomogeneous electro-chemical potentials. To start, we assume the following.

(H1) For all sufficiently small $X = (X_1, \ldots, X_M) \in \mathbb{R}^M$ there exists a unique state $\omega_X^{(0)}$ such that $\omega_X^{(0)}|_{\mathcal{O}_0}$ is (τ_0, β)-KMS and $\omega_X^{(0)}|_{\mathcal{O}_j}$ is $(\tau_j, \beta - X_j)$-KMS for $1 \leq j \leq M$.

Such a state correspond to each reservoir $\mathcal{R}_j$ being at equilibrium at inverse temperature $\beta_j = \beta - X_j$. The X_j's are the thermodynamic forces which drive the system out of equilibrium (see [Nonequilibrium steady states]). The conjugate fluxes are the energy currents $\Phi_j = \delta_j(V)$ (see [Entropy production]). To ensure that they are well defined we assume

(H2) $V \in \mathrm{Dom}(\delta_j)$ for $1 \leq j \leq M$.

It follows from Araki's perturbation theory (see [KMS states]) that $\omega_{X=0}^{(0)}$ (which is the unique $(\tau_{\mathrm{dec}}, \beta)$-KMS state) and ω are mutually normal. We note however that since $\omega_{X=0}^{(0)} \neq \omega$, expanding $\omega_X^{(0)} \circ \tau^t(A) - \omega(A)$ around $X = 0$ generates a spurious zeroth-order term. To avoid this problem we shall construct a family of states ω_X which on the one hand has the same thermodynamic properties as $\omega_X^{(0)}$ and on the other hand satisfies $\omega_{X=0} = \omega$.

By definition, the modular group of $\omega_X^{(0)}$ is generated by $-\beta\delta_{\rm dec} + \sum_{1\le j\le M} X_j\delta_j$. Denote by σ_X the group of $*$-automorphisms generated by

$$\zeta_X = -\beta\delta_{\rm dec} + \sum_{1\le j\le M} X_j\delta_j - {\rm i}\beta[V,\,\cdot\,] = \zeta + \sum_{j=1}^{M} X_j\delta_j.$$

Araki's perturbation theory implies that there exists a unique $(\sigma_X, -1)$-KMS state ω_X such that $\omega_X^{(0)}$ and ω_X are mutually normal. Thus, these two states have the same thermodynamic properties and since $\zeta_{X=0} = \zeta$ one also has $\omega_{X=0} = \omega$.

We say that $A \in \mathcal{O}$ is centered if $\omega_X(A) = 0$ for all sufficiently small $X \in \mathbb{R}^n$. The following result has been proven in [JOP1]

Theorem 1 *Under the Hypothesis (H1) and (H2), the function $X \mapsto \omega_X \circ \tau^t(A)$ is differentiable at $X = 0$ for any centered observable $A \in \mathcal{O}$ and the finite time Green-Kubo formula*

$$\partial_{X_j}\omega_X \circ \tau^t(A)|_{X=0} = \int_0^t \langle \tau^s(A)|\Phi_j\rangle_\omega \,{\rm d}s, \tag{3}$$

holds.

Remarks. 1. Formula (3) is limited to centered observables because, at the current level of generality, there is no way to control the behavior of $\omega_X(A)$ as $X \to 0$. If $A \in \mathcal{O}$ is such that $X \mapsto \omega_X(A)$ is differentiable at $X = 0$ then the above formula still holds after addition of the static contribution $\partial_{X_k}\omega_X(A)|_{X=0}$ to its right hand side. We note however that for infinite systems the states ω_X for distinct values of X are usually mutually singular. The differentiability of $\omega_X(A)$ is therefore a delicate question and is not expected to hold for general observables A.

2. One can prove that the energy fluxes Φ_j and more generally the fluxes conjugate to intensive thermodynamic parameters are centered. We refer to [JOP1] for more details.

2 The long time problem

The hard problem of linear response theory concerns the validity of the linear response formulas derived in the previous section in the long time limit. This delicate question has been largely discussed in the physics literature. The most famous objection to the validity of linear response was raised by van Kampen in [VK]. The basis of his argumentation is the fact that the microscopic dynamics of a large system, with many degrees of freedom, is strongly chaotic. He infers that the time scale on which a perturbative calculation remains valid can be very short. He concludes that the finite time linear response may well be physically irrelevant on a macroscopic time scale. A discussion of van Kampen's objection can be found in [KTH]. The interested reader should also consult [L].

A mathematical idealization reduces the long time problem to the interchange of two limits: The zero forcing limit involved in the derivation of the finite time linear response formulas and the infinite time limit. To illustrate this point let us continue the discussion of Subsection 1.2 which led us to Formula (3), assuming:

(H3) For all sufficiently small $X \in \mathbb{R}^M$ there exists a NESS ω_{X+} (see [NESS in quantum statistical mechanics]) such that,

$$\lim_{t\to\infty} \omega_X \circ \tau^t(A) = \omega_{X+}(A), \tag{4}$$

for any $A \in \mathcal{O}$.

Incidently we note that under such circumstances one expects more, namely that

$$\lim_{t\to\infty} \eta \circ \tau^t(A) = \omega_{X+}(A),$$

holds for any $A \in \mathcal{O}$ and any ω_X-normal (or equivalently $\omega_X^{(0)}$-normal) state η.

We shall say that the observable $A \in \mathcal{O}$ is regular if the function $X \mapsto \omega_{X+}(A)$ is differentiable at $X = 0$ and

$$\partial_{X_k}\omega_{X+}(A)|_{X=0} = \lim_{t\to\infty} \partial_{X_k}\omega_X \circ \tau^t(A)|_{X=0}.$$

If A is a regular, centered observable Equ. (4) and Formula (3) yield the Green-Kubo formula

$$\partial_{X_j}\omega_{X+}(A)|_{X=0} = \int_0^\infty \langle \tau^s(A)|\Phi_j\rangle_\omega \, \mathrm{d}s. \tag{5}$$

In particular, if the fluxes Φ_k are regular, then the transport coefficients (see [Nonequilibrium steady states]) defined by

$$\omega_{X+}(\Phi_k) = \sum_{1\le j\le M} L_{jk}X_j + \mathrm{o}(X),$$

are given by the formula

$$L_{jk} = \int_0^\infty \langle \tau^s(\Phi_k)|\Phi_j\rangle_\omega \, \mathrm{d}s.$$

To justify the exchange of limits for a sufficiently large set of centered observables $A \in \mathcal{O}$, in particular for the flux observables, is a delicate problem requiring a fairly good control on the dynamics of the system. This was recently achieved for two classes of systems: N-levels systems coupled to free Fermi reservoirs in [JOP2] and locally interacting Fermi gases in[JOP3]. In the first case the NESS was previously constructed in [JP] using the Liouvillean approach (see [NESS in quantum statistical mechanics]). In the second case, the NESS is obtained following Ruelle's scattering approach. In both cases, the interchange of limits is validated via the following simple consequence of Vitali's theorem.

Proposition 2 *Suppose that (H1) and (H3) hold and let $A \in \mathcal{O}$. Assume that for some $\epsilon > 0$ and any $t \ge 0$, the function $X \mapsto \omega_X \circ \tau^t(A)$ has an analytic extension to the open polydisk $D_\epsilon = \{X \in \mathbb{C}^M \mid \max_j |X_j| < \epsilon\}$. If*

$$\sup_{X\in D_\epsilon, t\ge 0} |\omega_X \circ \tau^t(A)| < \infty,$$

holds then A is regular.

It is evident but sometimes overlooked that the long time problem can not be solved by proving that a finite time linear response formula continues to make sense in the long time limit. Suppose for example that the system $(\mathcal{O}, \tau)$ is L^1-asymptotically Abelian, that is

$$\int_0^\infty \|[A, \tau^t(B)]\| \, \mathrm{d}t < \infty,$$

for any $A, B \in \mathcal{O}$. It follows that the linear response to the perturbation $V(t) = -\sum_j X_j(t)A_j$ such that $x = \sum_j \sup_t |X_j(t)| < \infty$ satisfies

$$(\Delta\omega)^t(A) = \lim_{s\to-\infty} (\Delta\omega)^{s\to t}(A) = \sum_j \int_0^\infty \omega(\mathrm{i}[A_j, \tau^u(A)])X_j(t-u) \, \mathrm{d}u, \tag{6}$$

where the integrals are absolutely convergent. This however does not mean that this formula is applicable, i.e., that (i) the natural nonequilibrium state

$$\omega_t^V(A) = \lim_{s\to-\infty} \omega \circ \tau_V^{s\to t}(A),$$

exists and (ii) that

$$\omega_t^V(A) - \omega(A) = (\Delta\omega)^t(A) + \mathsf{o}(x).$$

In fact both (i) and (ii) require a precise control of the perturbed dynamics τ_V whereas Equ. (6) only involves the unperturbed τ. If (i) and (ii) hold and if ω is (τ,β)-KMS then, by Equ. (2), the infinite time Green-Kubo formula

$$(\Delta\omega)^t(A) = \sum_j \beta \int_0^\infty \langle \tau^s(A)|\Phi_j\rangle_\omega \, X_j(t-s)\,\mathrm{d}s,$$

hold.

3 Time reversal invariance and Onsager reciprocity relations

A time reversal of $(\mathcal{O},\tau)$ is an involutive, antilinear $*$-automorphism Θ of $\mathcal{O}$ such that $\tau^t \circ \Theta = \Theta \circ \tau^{-t}$ for any $t \in \mathbb{R}$. A state ν on $\mathcal{O}$ is time reversal invariant if $\nu \circ \Theta(A) = \nu(A^*)$ for all $A \in \mathcal{O}$. An observable $A \in \mathcal{O}_{\mathrm{self}}$ is even/odd under time reversal whenever $\Theta(A) = \pm A$.

The following proposition is a simple consequence of the KMS condition (see [JOP1]).

Proposition 3 *Assume that $(\mathcal{O},\tau)$ is equipped with a time reversal Θ. Let ω be a time reversal invariant, mixing (τ,β)-KMS state. If $A, B \in \mathcal{O}_{\mathrm{self}}$ are both even or odd under time reversal then*

$$\int_0^t \langle \tau^s(A)|B\rangle_\omega \,\mathrm{d}s = \frac{1}{2}\int_{-t}^t \omega(A\tau^s(B))\,\mathrm{d}s + \mathrm{o}(1),$$

in the limit $t \to \infty$.

Remark. If ω is the unique (τ,β)-KMS state then it is automatically time reversal invariant.

To apply this proposition to the Green-Kubo formula (5) we assume:

(H4) $(\mathcal{O},\tau)$ is equipped with a time reversal Θ and ω is a time reversal invariant, mixing (τ,β)-KMS state. Moreover, the coupling V_j are even under time reversal.

Corollary 4 *Under Hypothesis (H1), (H2), (H3) and (H4) the Green-Kubo formula (5) can be written as*

$$\partial_{X_j}\omega_{X+}(A)|_{X=0} = \frac{1}{2}\int_{-\infty}^\infty \omega(A\tau^s(\Phi_j))\,\mathrm{d}s,$$

for regular, centered observables $A \in \mathcal{O}_{\mathrm{self}}$ which are odd under time reversal. In particular, if the fluxes Φ_k are regular then the transport coefficients are given by

$$L_{jk} = \frac{1}{2}\int_{-\infty}^\infty \omega(\Phi_k\tau^s(\Phi_j))\,\mathrm{d}s. \tag{7}$$

If ω is a mixing (τ,β)-KMS state then the stability condition

$$\int_{-\infty}^\infty \omega([A,\tau^t(B)])\,\mathrm{d}t = 0$$

holds for any $A, B \in \mathcal{O}$ (see [Stability and passivity of quantum states] or [BR2]). An important consequence of this fact and Equ. (7) is

Corollary 5 *Under the assumptions of Corollary 4 the transport coefficients satisfy the Onsager reciprocity relations*

$$L_{jk} = L_{kj}.$$

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