Linear Response Theory

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1 Response functions

We consider a time dependent Hamiltonian H, which is acted upon by an external time dependent field $F(t)$ which couple linearly to an observable B of the system:

$$H(t) = H_0 - AF(t) \tag{1}$$

at $t \leq t_0$, the system is in its groud state, at $t = t_0$ the external field is turned on and the system begin to evolve adiabatically. In the classical theory, the phase space probability ρ evolve as:

$$\frac{\partial \rho}{\partial t} = \{H(t), \rho\} \tag{2}$$

where $\{,\}$ is the poisson bracket. In linear approximation $\rho(t) = \rho_0 + \Delta\rho$, the equation of motion is:

$$\begin{aligned}\frac{\partial \rho(t)}{\partial t} &= \{H_0, \rho(t)\} + \{H', \rho_0\} \\ \frac{\partial \Delta\rho(t)}{\partial t} &= \{H_0, \Delta\rho(t)\} - \{A, \rho_0\}F(t)\end{aligned} \tag{3}$$

The change of the observed quantity B is given by:

$$\begin{aligned}\Delta B(t) &= \int dqdp \Delta\rho(t) B(q,p) \\ &= -\int dqdp \int_{-\infty}^{t} \{A, \rho_0\} B(t-t') F(t') dt'\end{aligned} \tag{4}$$

and the time dependence of operator B is given by the Heisenburg equation:

$$\dot{B}(p,q) = \{B, H_0\} \tag{5}$$

The response function is defined by the reponse of an observable after time t of a unit pulse:

$$\begin{aligned}\phi_{BA}(t) &= -\int dqdp \int_{-\infty}^{t} \{A, \rho_0\} B(t-t') \delta(t') dt' \\ &= -\int dqdp \{A, \rho_0\} B(t)\end{aligned} \tag{6}$$

so that

$$\Delta B(t) = \int_{-\infty}^{t} \phi_{BA}(t-t') F(t') dt' \tag{7}$$

which is summed over all the past time.

We define the frequency components of the response function as [1] :

$$\chi_{BA}(\omega) = \lim_{\eta \to 0^+} \int_0^{\infty} \phi_{BA}(t) e^{-\eta t - i\omega t} dt \tag{9}$$

[1] this follows the definition of *Kubo 1957* Eq.2.21, in terms of the more conventional way, we have:

$$\chi_{BA}(\omega) = \lim_{\eta \to 0^+} \int_0^{\infty} \phi_{BA}(t) e^{i(\omega + i\eta)\tau} dt \tag{8}$$

Let's consider the case where a (constant pertrubation) F is applied continuously from $t = -\infty$ to $t = 0$ and stops. The system then relax throught internal interaction. The observable will follow:

$$\begin{aligned}\Delta B(t) &= \int_{-\infty}^{0} \phi_{BA}(t-t')dt'F \\ &= \int_{t}^{\infty} \phi_{BA}(t')dt'F \\ &= \Phi_{BA}(t)F \end{aligned} \tag{10}$$

and

$$\Phi_{BA}(t) = \lim_{\eta\to 0^+} \int_t^{\infty} \phi_{BA}(t')e^{-\eta t'}dt' \tag{11}$$

2 Response functions in Quantum case

In quantum case, the evolution of density matrix ρ is given by:

$$\frac{d}{dt}\rho'(t) = \frac{1}{i\hbar}[H(t), \rho'(t)] \tag{12}$$

$$\rho'(t) = \rho_0 + \Delta\rho(t) \tag{13}$$

and

$$\phi_{BA}(t) = -\frac{1}{i\hbar}\mathrm{Tr}\int_{-\infty}^{t}[A, \rho_0]B(t-t')\delta(t')dt' \tag{14}$$

with the time dependence of B given by:

$$\dot{B}(t) = \frac{1}{i\hbar}[B(t), H_0] \tag{15}$$

with $B(0) = B$ in the Schrodinger's picture.

$$\phi_{BA}(t) = \frac{1}{i\hbar}\mathrm{Tr}[\rho_0, A]B(t) \tag{16}$$

$$= \frac{1}{i\hbar}\mathrm{Tr}\rho_0[A, B(t)] \tag{17}$$

$$= \frac{1}{i\hbar}\langle[A, B(t)]\rangle_0 \tag{18}$$

We can find the following relationship:

$$[\rho_0, A] = i\hbar\int_0^{\beta}\rho_0\dot{A}(-i\hbar\lambda)d\lambda \tag{19}$$

So that we can express:

$$\phi_{BA}(t) = \int_0^{\beta}\mathrm{Tr}\rho_0\dot{A}(-i\hbar\lambda)B(t)d\lambda \tag{20}$$

$$\chi_{BA}(\omega) = \lim_{\eta\to 0^+}\int_0^{\beta}d\lambda\int_0^{\infty}e^{-\eta t - i\omega t}dt\mathrm{Tr}\rho_0\dot{A}(-i\hbar\lambda)B(t) \tag{21}$$

3 Linear response formula of conductivity

We consider an uniform external electric field (potential zero is arbitrary):

$$H'(t) = -e\sum_i x_i E(t) = -AE(t) \tag{22}$$

$$\dot{A} = e\sum_i \dot{x}_i = J \tag{23}$$

where x_i is the position operator of the i^{th} particle. The current operator is defined to be:

$$J_\mu = e\sum_i \dot{x}_i \tag{24}$$

The response function is given by:

$$\phi_{\mu\nu}(t) = \int_0^\beta \langle J_\nu(-i\hbar\lambda)J_\mu(t)\rangle_0 d\lambda \tag{25}$$

$$\chi_{\mu\nu}(\omega) = \lim_{\eta\to 0^+}\int_0^\beta d\lambda \int_0^\infty e^{-\eta t - i\omega t} dt \langle J_\nu(-i\hbar\lambda)J_\mu(t)\rangle_0 \tag{26}$$

and the conductivity is given by:

$$\sigma_{\mu\nu} = \int_0^\beta d\lambda \int_0^\infty dt \langle J_\nu(-i\hbar\lambda)J_\mu(t)\rangle_0 \tag{27}$$

4 From Q.T.E.L.

The time evolution of the system is given by:

$$
\begin{aligned}
|\Psi_n(t)\rangle &= U(t,t_0)|\Psi_n(t_0)\rangle \\
&= e^{-\frac{i}{\hbar}H_0(t-t_0)}U_I(t,t_0)|\Psi_n(t_0)\rangle
\end{aligned}
$$

$U_I(t,t_0)$ is given by the equation of motion:

$$
i\hbar\frac{\partial}{\partial t}U_I(t,t_0) = f(t)B(t-t_0)U_I(t,t_0) \tag{28}
$$

with the initial condition $U_I(t_0,t_0) = 1$. Making the approximation that $U_I(t,t_0) = 1$ on the right hand side of the Eq.28 and integrate from time $t_0 \to t$, we obtain the first order approximation:

$$
U_I^{(1)}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} f(t')B(t'-t_0)dt' \tag{29}
$$

The thermal average of another observable of the system A is given by:

$$
\langle A\rangle_0 = \frac{1}{Z}\sum_n e^{-\beta E_n}\langle\Psi_n(t_0)|A|\Psi_n(t_0)\rangle \tag{30}
$$

and since we consider adiabatic evolution, at a later time t, the thermal average is given by:

$$
\langle A\rangle(t) = \frac{1}{Z}\sum_n e^{-\beta E_n}\langle\Psi_n(t)|A|\Psi_n(t)\rangle \tag{31}
$$

where the probability of finding each state is kept constants (instead of $e^{-\beta H}$ as an operator). Now, inserting the evolution of states, we obtain:

$$
\langle A\rangle(t) - \langle A\rangle_0 = -\frac{i}{\hbar}\int_{t_0}^{t}\langle[A(t),B(t')]\rangle_0 f(t')dt' \tag{32}
$$

where is thermal average is taken at the time independent equilibrium ensemble, and the time dependence of the operator $A(t)$ and $B(t)$ is given by the Heisenburg form:

$$
B(t) = e^{\frac{i}{\hbar}H_0 t}Be^{-\frac{i}{\hbar}H_0 t} \tag{33}
$$

taking $\tau = t - t' > 0$, we can define:

$$
\chi_{AB}(\tau) = -\frac{i}{\hbar}\theta(\tau)\langle[A(\tau),B]\rangle_0 \tag{34}
$$

so that

$$
\langle A\rangle(t) = \langle A\rangle_0 + \int_0^{t-t_0}\chi_{AB}(\tau)f(t-\tau)d\tau \tag{35}
$$

where we changed the integral variable from t' to $\tau = t - t'$.

Because of the $\theta(\tau)$ in Eq.34, $\chi_{AB}(\tau)$ is called the retarded response function. We have previously taken the external field to turn on instantly at t_0, however, if we allow the field to switch on slowly, as $f(t) \to 0$ as $t_0 \to -\infty$, the result at time t should remain the same, so we can also take:

$$
\langle A\rangle(t) = \langle A\rangle_0 + \int_0^{\infty}\chi_{AB}(\tau)f(t-\tau)d\tau \tag{36}
$$

5 Frequency domain

Consider a switching on (real) periodic perturbation, which vanish for $t \to -\infty$:

$$
f(t) = f_\omega e^{-i(\omega+i\eta)t} + c.c. \tag{37}
$$

η is a positive and η^{-1} give a time scale that longer than period of the perturbation. We can thus apply the linear response formalism and take the limit $\eta \to 0^+$ at the end of the calculation. If this limit exist, it should describe the reponse of the system to a steady periodic field that has been applied long enough so that initial condition is ignorable.

Inserting the periodic perturbation into Eq.36 gives:

$$\langle A\rangle(t) - \langle A\rangle_0 = \chi_{AB}(\omega) f_\omega e^{-i\omega t} + c.c. \tag{38}$$

where

$$\chi_{AB}(\omega) = -\frac{i}{\hbar} \lim_{\eta\to 0^+} \int_0^\infty \langle [A(\tau), B]\rangle_0 e^{i(\omega+i\eta)\tau} d\tau \tag{39}$$

For any general perturbation, we fourier transform between t and ω is given by:

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega) e^{i\omega t} d\omega \tag{40}$$

$$f(\omega) = \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt \tag{41}$$