Linear Response Theory

Wenhao

August 18, 2021

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:

$$H(t) = H_0 + f(t)B \tag{1}$$

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. 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:

$$i\hbar\frac{\partial}{\partial t}U_I(t,t_0) = f(t)B(t-t_0)U_I(t,t_0) \tag{2}$$

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.2 and integrate from time $t_0 \to t$, we obtain the first order approximation:

$$U_I^{(1)}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} f(t')B(t'-t_0)dt' \tag{3}$$

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

$$\langle A\rangle_0 = \frac{1}{Z}\sum_n e^{-\beta E_n}\langle\Psi_n(t_0)|A|\Psi_n(t_0)\rangle \tag{4}$$

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

$$\langle A\rangle(t) = \frac{1}{Z}\sum_n e^{-\beta E_n}\langle\Psi_n(t)|A|\Psi_n(t)\rangle \tag{5}$$

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:

$$\langle A\rangle(t) - \langle A\rangle_0 = -\frac{i}{\hbar}\int_{t_0}^{t}\langle[A(t),B(t')]\rangle_0 f(t')dt' \tag{6}$$

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:

$$B(t) = e^{\frac{i}{\hbar}H_0 t}Be^{-\frac{i}{\hbar}H_0 t} \tag{7}$$

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

$$\chi_{AB}(\tau) = -\frac{i}{\hbar}\theta(\tau)\langle[A(\tau),B]\rangle_0 \tag{8}$$

so that

$$\langle A\rangle(t) = \langle A\rangle_0 + \int_0^{t-t_0} \chi_{AB}(\tau) f(t-\tau) d\tau \tag{9}$$

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

Because of the $\theta(\tau)$ in Eq.8, $\chi_{AB}(\tau)$ 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:

$$\langle A\rangle(t) = \langle A\rangle_0 + \int_0^{\infty} \chi_{AB}(\tau) f(t-\tau) d\tau \tag{10}$$

2 Frequency domain

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

$$f(t) = f_\omega e^{-i(\omega+i\eta)t} + c.c. \tag{11}$$

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.10 gives:

$$\langle A\rangle(t) - \langle A\rangle_0 = \chi_{AB}(\omega) f_\omega e^{-i\omega t} + c.c. \tag{12}$$

where

$$\chi_{AB}(\omega) = -\frac{i}{\hbar} \lim_{\eta\to 0^+} \int_0^{\infty} \langle [A(\tau), B]\rangle_0 e^{i(\omega+i\eta)\tau} d\tau \tag{13}$$

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

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega) e^{i\omega t} d\omega \tag{14}$$

$$f(\omega) = \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt \tag{15}$$