II. Linear response theory

· Linear response to an external potential

Consider a system described by a time-independent Hamiltonian $\hat{H}$, which is perturbed by a time dependent perturbation $\hat{V}(t)$:

$$\hat{H}_{tot}(t) = \hat{H} + \hat{V}(t)$$

Question: For an observable $\hat{A}$, evaluate $\langle \hat{A}(t) \rangle_{tot}$ up to first order in $\hat{V}(t)$?

For $\hat{V}(t)=0$, $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(0)\rangle$ with

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle.$$

For $\hat{V}(t) \neq 0$, assume that

$$|\psi(t)\rangle_{tot} = e^{-\frac{i}{\hbar}\hat{H}t}\hat{O}_{ext}(t)|\psi(0)\rangle$$ with

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle_{tot} = \hat{H}_{tot}(t)|\psi(t)\rangle_{tot}$$

$$\rightarrow \underbrace{i\hbar\frac{\partial}{\partial t}\left(e^{-\frac{i}{\hbar}\hat{H}t}\hat{O}_{ext}(t)|\psi(0)\rangle\right)} = \left(\hat{H}+\hat{V}(t)\right)e^{-\frac{i}{\hbar}\hat{H}t}\hat{O}_{ext}(t)|\psi(0)\rangle$$

$$e^{-\frac{i}{\hbar}\hat{H}t}\left(\hat{H}\hat{O}_{ext}(t) + i\hbar\frac{\partial}{\partial t}\hat{O}_{ext}(t)\right)|\psi(0)\rangle$$

$$\rightarrow i\hbar \frac{\partial}{\partial t}\hat{O}_{ext}(t) = \hat{V}_H(t)\hat{O}_{ext}(t)$$

$$\hat{V}_H(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}t}$$ H: Heisenberg picture for $\hat{H}$

Thus, up to first order in $\hat{V}(t)$,

$$\hat{O}_{ext}(t) \approx 1 - \frac{i}{\hbar}\int_0^t dt' \hat{V}_H(t')$$

$(|\psi_H\rangle = |\psi(0)\rangle)$

$$\therefore \langle\psi_{tot}(t)|\hat{A}(t)|\psi_{tot}(t)\rangle = \langle\psi_H|\hat{O}^{\dagger}_{ext}(t)\hat{A}_H(t)\hat{O}_{ext}(t)|\psi_H\rangle$$

$$\approx \langle\psi_H|\left(1+\frac{i}{\hbar}\int_0^t dt' \hat{V}_H(t')\right)\hat{A}_H(t)\left(1-\frac{i}{\hbar}\int_0^t dt' \hat{V}_H(t')\right)|\psi_H\rangle$$

$$\approx \langle\psi(t)|\hat{A}(t)|\psi(t)\rangle$$

$$-\frac{i}{\hbar}\int_0^t dt' \langle\psi_H|[\hat{A}_H(t), \hat{V}_H(t')]|\psi_H\rangle$$

Assume that the external perturbation is given by an external (time-dependent) field $F(t)$ coupled linearly to an observable $\hat{B}(t)$; $\hat{V}(t) = \hat{B}(t)F(t)$.

$$\delta\langle A(t)\rangle = \langle\psi_{tot}(t)|\hat{A}(t)|\psi_{tot}(t)\rangle - \langle\psi(t)|\hat{A}(t)|\psi(t)\rangle$$

$$\approx \int_0^{\infty} dt' \chi_{AB}(t-t')F(t')$$

$$i\hbar\chi_{AB}(t-t') = \Theta(t-t')\langle\psi_H|[\hat{A}_H(t), \hat{B}_H(t')]|\psi_H\rangle$$

- Here $\chi_{AB}(t-t')$ describes the response of the observable $\hat{A}$ at a time t to an external perturbation that couples to the observable $\hat{B}$ through the external field F at an earlier time $t'<t$. Note $\chi_{AB}(t<0) = 0$ due to causality.
- Thus, the linear response of a system to an external potential is characterized by the retarded (causal) correlation function, which is intrinsic properties of the unperturbed system.
- The linear response theory links a response measured experimentally and a correlation calculated theoretically.
- Many important physical properties can be evaluated from various types of correlation functions.

If the system Hamiltonian does not explicitly depend on time, $\chi_{AB}(t,t') = \chi_{AB}(t-t')$.

After Fourier transformation,

$$\delta\langle A(\omega)\rangle = \chi_{AB}(\omega) F(\omega)$$

Note that in a linear response regime, a perturbation at a certain frequency will cause a response of the same frequency.

- Density response to a scalar potential

Consider a density response to a scalar potential V_{ext} that couples linearly to the density $\hat{\rho}(x,t)$

$$\hat{V}(t) = \int dx\, \hat{\rho}(x,t) V_{ext}(x,t)$$

$$\rightarrow \delta\langle\hat{\rho}(x,t)\rangle = \int dx' \int dt' \chi(x,x';t-t') V_{ext}(x',t')$$

For a homogeneous system, $\chi(x, x'; t-t') = \chi(x-x'; t-t')$

Then after Fourier transform with respect to x,

$$\delta\langle\hat{\rho}(q, t)\rangle = \int dt' \chi(q, t-t') V_{ext}(q, t')$$

$$i\hbar\chi(q, t-t') = \frac{1}{V}\Theta(t-t')\langle[\hat{\rho}(q, t), \hat{\rho}(-q, t')]\rangle$$

$$\hat{\rho}(q) = \sum_{k,\sigma} \hat{a}^{\dagger}_{k+q,\sigma} a_{k,\sigma}$$

After Fourier transform with respect to t,

$$\delta\langle\hat{\rho}(q, \omega)\rangle = \chi(q, \omega) V_{ext}(q, \omega)$$

Thus, in the linear response regime, a perturbation with q, ω causes a response with the same q, ω.

· Density response of noninteracting electrons

$$i\hbar\chi_0(q, t) = \frac{\Theta(t)}{V}\langle[\hat{\rho}(q, t), \hat{\rho}(-q, 0)]\rangle$$

$$\hat{a}_{k\sigma}(t) = e^{-i\omega_k t}\hat{a}_{k\sigma}, \quad \hat{a}^{\dagger}_{k\sigma}(t) = e^{i\omega_k t}\hat{a}^{\dagger}_{k\sigma}$$

$$i\hbar\chi_0(q,t) = \frac{\Theta(t)}{V}\sum_{k,k',\sigma,\sigma'}\left\langle\left[a^\dagger_{k+q,\sigma'}a_{k,\sigma'}e^{i(\omega_{k+q}-\omega_k)t}, a^\dagger_{k+q,\sigma}a_{k,\sigma}\right]\right\rangle$$

$$= \frac{\Theta(t)}{V}\sum_{k\sigma}\left\langle \hat{a}^\dagger_{k,\sigma}\hat{a}_{k,\sigma} - \hat{a}^\dagger_{k+q,\sigma}\hat{a}_{k+q,\sigma}\right\rangle e^{i(\omega_k-\omega_{k+q})t}$$

Note $[\hat{a}^\dagger_\alpha\hat{a}_\beta, \hat{a}^\dagger_\gamma\hat{a}_\delta] = \delta_{\beta\gamma}\hat{a}^\dagger_\alpha\hat{a}_\beta - \delta_{\alpha\delta}\hat{a}^\dagger_\gamma\hat{a}_\beta$

for both bosons and fermions.

After Fourier transform with respect to t,

$$\chi_0(q,\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\chi_0(q,t)$$

$$= \frac{1}{i\hbar V}\sum_{k,\sigma}\int_0^\infty dt\, e^{i(\omega+\omega_k-\omega_{k+q})t}(f_{k,\sigma}-f_{k+q,\sigma})$$

$$= -\frac{1}{\hbar V}\sum_{k\sigma}\frac{e^{i(\omega+\omega_k-\omega_{k+q}+i\eta)}}{\omega+\omega_k-\omega_{k+q}+i\eta}\Bigg|_0^\infty(f_{k\sigma}-f_{k+q,\sigma})$$

$$\overset{f_{k\sigma}=f_k}{=} g_s\int\frac{d^dk}{(2\pi)^d}\frac{f_k-f_{k+q}}{\hbar\omega+\epsilon_k-\epsilon_{k+q}+i\eta}$$

where $f_k = \langle a^\dagger_{k,\sigma}a_{k,\sigma}\rangle \to \frac{1}{e^{\beta(\epsilon_k-\mu)}+1}$

$g_s = \sum_\sigma = 2$ is the spin degeneracy factor and

$\eta = 0^+$ is a positive infinitesimal number.

Here, the $i\eta$ term is associated with causality of the response function. In general, due to causality, a response function in frequency space is analytic in the upper half of the complex frequency planes and has poles only in the lower half. This close connection between the causality and analyticity leads to the Kramers–Kronig relation.

Further reading: Giuliani & Vignale, Ch. 3.2.7

Note that

$$\chi_0(q \to 0, \omega = 0) = g_s \int \frac{d^d k}{(2\pi)^d} \frac{\partial f_k}{\partial \varepsilon_k} \xrightarrow{T=0} -N_0$$

where N_0 is the density of states per unit volume at the Fermi energy, thus a measure of excited states available to the system for vanishing excitation energy.

· Density response of interacting electrons

When an electron gas is perturbed by an external potential $v_{ext}(x;t)$, the change in density $\delta\rho(x';t)$ generates a Coulomb potential $v_c(x-x')$, and the resulting screened potential is given by

$$v_{scr}(x;t) = v_{ext}(x;t) + \int dx'\, v_c(x-x')\,\delta\rho(x';t), \text{ or}$$

in momentum-frequency space.

$$v_{scr}(q,\omega) = v_{ext}(q,\omega) + v_c(q)\,\delta\rho(q,\omega)$$

Then to linear order, the response is given by

$$\chi = \frac{\delta\rho}{\delta v_{ext}} = \frac{\delta\rho}{\delta v_{scr}}\frac{\delta v_{scr}}{\delta v_{ext}} = \chi^{\star}\left(1 + v_c\frac{\delta\rho}{\delta v_{ext}}\right)$$

$$= \chi^{\star} + \chi^{\star} v_c \chi = \frac{\chi^{\star}}{1 - v_c\chi^{\star}} \quad \text{or} \quad \chi^{-1} = (\chi^{\star})^{-1} - v_c$$

where $\chi^{\star} = \frac{\delta\rho}{\delta v_{scr}}$ is called the proper response function which describes a response of the screened field.

The dielectric function is defined by $\epsilon^{-1} = \frac{\delta V_{scr}}{\delta V_{ext}}$

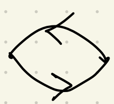
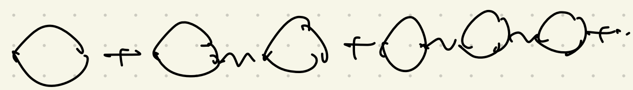
From $\delta\rho = \chi\,\delta V_{ext} = \chi^*\,\delta V_{scr}$, $\chi = \frac{\chi^*}{1 - v_c\chi^*}$ or $\chi^{-1} = (\chi^*)^{-1} - v_c$

$$\epsilon^{-1} = \frac{\delta V_{scr}}{\delta V_{ext}} = \frac{\chi}{\chi^*} = 1 + v_c\chi \quad \text{or} \quad \epsilon = 1 - v_c\chi^*$$

The approximation $\chi^* = \chi_0$ is called the random phase approximation (RPA). In RPA,

$\epsilon^{RPA} = 1 - v_c\chi_0$ and

$$\chi^{RPA} = \frac{\chi_0}{1 - v_c\chi_0} = \chi_0 + \chi_0 v_c \chi_0 + \chi_0 v_c \chi_0 v_c \chi_0 + \cdots$$

$\chi_0 =$  $\chi^{RPA} =$ 

Diagramatically, the RPA corresponds to an infinite series of bubble diagrams connected by bare interaction lines neglecting other higher order terms, which is known to be valid in the weak coupling (typically high density) limit or in the large fermion flavor (or large N) limit.

→ screening, collective modes, correlation, ...

Further reading: Giuliani & Vignale. Ch.3~Ch.5