Chap 3 Linear response theory

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I. GENERAL FORMULATION

A material would polarize, or carry a current under an external electric field,

$$\begin{aligned} \mathbf{P} &= \chi_e \mathbf{E} \\ \mathbf{j} &= \sigma \mathbf{E}. \end{aligned} \tag{1}$$

If the electric field is not too strong, then the electric susceptibility and the conductivity are independent of the electric field. They only depend on the material properties *in the absence* of the electric field (in equilibrium). This type of response is called the linear response.

The average of an observable (such as the electric polarization) in equilibrium is

$$\langle A \rangle_0 = \frac{1}{Z_0} \sum_{\{n\}^0} e^{-\beta E_{\{n\}^0}} \langle \{n\}^0 | A | \{n\}^0 \rangle. \tag{2}$$

Under an external field, the states $\{n\}^0$ are perturbed to become $\{n\}$, and the average becomes

$$\langle A \rangle = \frac{1}{Z} \sum_{\{n\}} e^{-\beta E_{\{n\}}} \langle \{n\} | A | \{n\} \rangle = \langle A \rangle_0 + \delta \langle A \rangle. \tag{3}$$

Our job is to find out $\delta\langle A \rangle$.

In the following, as long as there is no ambiguity, we will write the labels of a manybody state $\{n\}$ simply as n. Before perturbation,

$$H_0 | n^0 \rangle = E_n^0 | n^0 \rangle, \tag{4}$$

where E_n^0 and $|n^0\rangle$ are eigne-energies and eigenstates of the manybody Hamiltonian H_0. The external perturbation is assumed to be

$$H = H_0 + H'(t)\theta(t - t_0). \tag{5}$$

That is, the perturbation is turned on at time t_0. After the perturbation,

$$H(t)|n(t)\rangle = i \frac{\partial}{\partial t} |n(t)\rangle. \tag{6}$$

In the **interaction picture**, the perturbed states

$$\begin{aligned} |n(t)\rangle &= e^{-iH_0 t} |n_I(t)\rangle \\ &= e^{-iH_0 t} U_I(t, t_0) |n_I(t_0)\rangle, \end{aligned} \tag{7}$$

where

$$U_I(t, t_0) = 1 - i \int_{t_0}^{t} dt' H_I'(t') + \cdots, \tag{8}$$

and $|n_I(t_0)\rangle = |n^0\rangle$ is the states before perturbation.

Substitute Eqs. (7) and (8) into Eq. (3), and keep only the terms to linear order in H', we have

$$\begin{aligned} &\langle A(t) \rangle \\ &= \langle A \rangle_0 - i \int_{t_0}^{t} dt' \sum_n \langle n^0 | [A_I(t), H_I'(t')] | n^0 \rangle \frac{e^{-\beta E_n^0}}{Z_0} \\ &= \langle A \rangle_0 - i \int_{t_0}^{t} dt' \langle [A_I(t), H_I'(t')] \rangle_0. \end{aligned} \tag{9}$$

For example, if

$$H'(t) = \int dv \underbrace{\mathbf{B}(\mathbf{r})}_{\text{operator}} \cdot \underbrace{\mathbf{f}(\mathbf{r}, t)}_{C-\text{number}}, \tag{10}$$

then

$$\begin{aligned} &\delta \langle A(\mathbf{r}, t) \rangle \\ &= -i \int dv' \int_{t_0}^{t} dt' \langle [A_I(\mathbf{r}, t), \mathbf{B}_I(\mathbf{r}', t')] \rangle_0 \cdot \mathbf{f}(\mathbf{r}', t') \\ &= -i \int dv' \int_{-\infty}^{\infty} dt' \theta(t - t') \langle [A_I(\mathbf{r}, t), \mathbf{B}_I(\mathbf{r}', t')] \rangle_0 \cdot \mathbf{f}(\mathbf{r}', t'), \end{aligned} \tag{11}$$

This can be written as

$$\delta \langle A(x) \rangle = \int dx' \sum_\alpha \chi_{AB_\alpha}(x, x') f_\alpha(x'), \tag{12}$$

where $x = (\mathbf{r}, t)$, $dx' \equiv dv'dt'$, and

$$\chi_{AB_\alpha}(x, x') = -i\theta(t - t') \langle [A_I(x), B_{I\alpha}(x')] \rangle_0. \tag{13}$$

Eq (12) is called the **Kubo formula**, and χ_{AB_α} is called the **response function**. Notice that the operators are written in the interaction picture.

II. DENSITY RESPONSE AND DIELECTRIC FUNCTION

A. Density response

In this section, we consider the perturbation of electron density caused by an external electric potential. Before perturbation,

$$H_0 = T + V_L + V_{ee}, \tag{14}$$

where V_L is a one-body interaction, such as the electron-ion interaction, and V_{ee} is the electron-electron interaction. The perturbation can be written in the following form,

$$H' = \int dv \rho_e(\mathbf{r})\phi_{ext}(\mathbf{r},t), \tag{15}$$

where $\rho_e = q\sum_s \psi_s^\dagger(\mathbf{r})\psi_s(\mathbf{r})$ ($q=-e$) is the electron density, and ϕ_{ext} is an external potential.

Because of the external potential ϕ_{ext}, electron density

$$\langle\rho_e\rangle_0 \to \langle\rho_e\rangle = \langle\rho_e\rangle_0 + \delta\langle\rho_e\rangle. \tag{16}$$

Comparing with the Kubo formula, we find the following replacement necessary,

$$\begin{aligned} A &\to \rho_e, \\ \mathbf{B} &\to \rho_e, \\ \mathbf{f} &\to \phi_{ext}. \end{aligned} \tag{17}$$

The Kubo formula gives

$$\delta\langle\rho_e(x)\rangle = \int dx' \chi_{\rho_e}(x,x')\phi(x'), \tag{18}$$

and the response function is

$$\chi_{\rho_e}(x,x') = -i\theta(t-t')\langle[\rho_e(x),\rho_e(x')]\rangle_0. \tag{19}$$

Remember that the operators are in the interaction picture, but the subscript I is neglected from now on.

If the unperturbed system H_0 is uniform in both space and time, then

$$\chi_{\rho_e}(x,x') = \chi_{\rho_e}(x-x'). \tag{20}$$

In this case, the convolution theorem in Fourier analysis tells us that

$$\delta\langle\rho_e(\kappa)\rangle = \chi_{\rho_e}(\kappa)\phi_{ext}(\kappa) \tag{21}$$

where $\kappa \equiv (\mathbf{q},\omega)$, $\kappa x \equiv \mathbf{q}\cdot\mathbf{r} - \omega t$, and

$$\begin{aligned} \delta\langle\rho_e(x)\rangle &= \sum_\kappa e^{i\kappa x}\delta\langle\rho_e(\kappa)\rangle, \\ \delta\langle\rho_e(\kappa)\rangle &= \int dx e^{-i\kappa x}\delta\langle\rho_e(x)\rangle; \\ \phi_{ext}(x) &= \sum_\kappa e^{i\kappa x}\phi_{ext}(\kappa), \\ \phi_{ext}(\kappa) &= \int dx e^{-i\kappa x}\phi_{ext}(x). \end{aligned} \tag{22}$$

The summation over k should be understood as

$$\sum_\kappa = \frac{1}{V_0}\sum_{\mathbf{q}}\int\frac{d\omega}{2\pi}. \tag{23}$$

The Fourier expansion of the response function is

$$\chi_{\rho_e}(x-x') = \sum_\kappa e^{i\kappa(x-x')}\chi_{\rho_e}(\kappa), \tag{24}$$

and

$$\begin{aligned} \chi_{\rho_e}(\kappa) &= \int d(x-x')e^{-i\kappa(x-x')}\chi_{\rho_e}(x-x') \\ &= -i\int d(t-t')\theta(t-t')e^{i\omega(t-t')} \\ &\times \int d(\mathbf{r}-\mathbf{r}')e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\langle[\rho_e(\mathbf{r},t),\rho_e(\mathbf{r}',t')]\rangle_0. \end{aligned} \tag{25}$$

Since the system is uniform in space, one can perform an extra space integral $\frac{1}{V_0}\int dr'$ to the space integral above, and use

$$\frac{1}{V_0}\int dr'\int d(\mathbf{r}-\mathbf{r}') = \frac{1}{V_0}\int dr\int dr'. \tag{26}$$

Then it is not difficult to see that

$$\chi_{\rho_e}(\kappa) = -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}\langle[\rho_e(\mathbf{q},t),\rho_e(-\mathbf{q},0)]\rangle_0. \tag{27}$$

Notice that $\rho_e(-\mathbf{q},0)$ can also be written as $\rho_e^\dagger(\mathbf{q},0)$. In the following, we may sometimes use the particle density ρ and its response function χ_ρ, which are related to the electron density and its response function as

$$\rho_e = -e\rho, \quad \chi_{\rho_e} = e^2\chi_\rho. \tag{28}$$

Also, notice that these response functions are related to, but not exactly the same as, the electric susceptibility χ_e introduced at the beginning of this chapter.

B. Dielectric function

The response function connects $\delta\rho_e$ with ϕ_{ext}. However, the dielectric function connects ϕ_{ext} with the total potential ϕ, which is the sum of ϕ_{ext} and the potential due to material response,

$$\epsilon(\kappa) = \frac{\phi_{ext}(\kappa)}{\phi(\kappa)}. \tag{29}$$

The total particle density is

$$\langle\rho\rangle = \langle\rho\rangle_{ext} + \delta\langle\rho\rangle, \tag{30}$$

which are related to the potentials via the Poisson equations (CGS),

$$\begin{aligned} q^2\phi_{ext}(\kappa) &= -4\pi e\langle\rho(\kappa)\rangle_{ext}, \\ q^2\phi(\kappa) &= -4\pi e\langle\rho(\kappa)\rangle. \end{aligned} \tag{31}$$

Notice that quantities such as $\phi_{ext}(\kappa) = \phi_{ext}(\mathbf{q},\omega)$ is allowed to be frequency-dependent. Also, if one prefers the MKS system, then just replaces 4π with $\frac{1}{\epsilon_0}$.

Combine the equations above, we get

$$\phi(\kappa) = \phi_{ext} + 4\pi e^2\chi_\rho\frac{\phi_{ext}}{q^2}. \tag{32}$$

This leads to

$$\frac{1}{\epsilon(\kappa)} = 1 + \underbrace{\frac{4\pi e^2}{q^2}}_{V^{(2)}(\mathbf{q})} \chi_\rho, \tag{33}$$

in which $V^{(2)}(\mathbf{q})$ is the Fourier transform of $V^{(2)}(\mathbf{r}) = e^2/r$.

Instead of using $\delta\langle\rho\rangle = \chi_\rho \phi_{ext}$, an alternative relation is

$$\delta\langle\rho\rangle = \chi_\rho^0 \phi, \quad \phi = \phi_{ext} + \delta\phi. \tag{34}$$

It's not difficult to see that

$$\chi_\rho = \frac{\chi_\rho^0}{1 - \frac{4\pi e^2}{q^2}\chi_\rho^0}, \tag{35}$$

and

$$\epsilon(\kappa) = 1 - \frac{4\pi e^2}{q^2}\chi_\rho^0. \tag{36}$$

The calculation of χ_ρ is based on Eq. (27), in which one averages over *unperturbed* manybody states (*including* electron interactions). A great advantage of using the alternative response function χ_ρ^0 is that, since the local field correction has been included in ϕ, one may use *non-interacting* manybody states in the calculation of the response function. This is justified as follows:

The interaction term is, apart from a one-body correction (see Sec. IV.B.1 of Chap 1),

$$V_{ee} = \frac{1}{2}\int dv dv' V^{(2)}(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r})\rho_e(\mathbf{r}'). \tag{37}$$

Using the mean field approximation, and expand the charge density with respect to a mean value $\langle\rho(\mathbf{r})\rangle_e$,

$$\rho_e(\mathbf{r}) = \langle\rho_e(\mathbf{r})\rangle + \underbrace{\rho_e(\mathbf{r}) - \langle\rho_e(\mathbf{r})\rangle}_{\delta\rho_e(\mathbf{r})}. \tag{38}$$

Neglecting the $(\delta\rho_e)^2$ term, we have

$$\begin{aligned} V_{ee} \simeq & \int dv dv' V^{(2)}(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r})\langle\rho_e(\mathbf{r}')\rangle \\ & - \frac{1}{2}\int dv dv' V^{(2)}(\mathbf{r}-\mathbf{r}')\langle\rho_e(\mathbf{r})\rangle\langle\rho_e(\mathbf{r}')\rangle. \end{aligned} \tag{39}$$

The mean-field Hamiltonian under perturbation is (dropping the second term in Eq. (39))

$$\begin{aligned} & H_{MF} \\ = & \tilde{H}_0 + \int dv dv' V^{(2)}(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r})\langle\rho_e(\mathbf{r}')\rangle + \int dv \rho_e(\mathbf{r})\phi_{ext} \\ = & \tilde{H}_0 + \int dv \rho_e(\mathbf{r})\phi(\mathbf{r}), \end{aligned} \tag{40}$$

where $\tilde{H}_0 = T + V_L$, and

$$\phi(\mathbf{r}) = \phi_{ext}(\mathbf{r}) + \int dv' V^{(2)}(\mathbf{r}-\mathbf{r}')\langle\rho_e(\mathbf{r}')\rangle. \tag{41}$$

The second term in $\phi(\mathbf{r})$ is the induced potential, or the local field correction. That is, if one calculates the response to the total perturbing potential $\phi(\mathbf{r})$, then the unperturbed system is $\tilde{H}_0$, which is non-interacting.

C. Calculation of χ_ρ^0

We now drop the superscript and subscript 0 that refer to equilibrium states. Recall that

$$\chi_\rho^0(\kappa) = -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}\langle[\rho(\mathbf{q},t),\rho(-\mathbf{q},0)]\rangle. \tag{42}$$

In the interaction picture, $\rho(\mathbf{q},t) = e^{iH_0 t}\rho(\mathbf{q})e^{-iH_0 t}$. The summation

$$\begin{aligned} & I(\mathbf{q};t,0) \\ \equiv & \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|\rho(\mathbf{q},t)\rho(-\mathbf{q},0)|n\rangle \\ = & \sum_{n,m}\frac{e^{-\beta E_n}}{Z} e^{i(E_n-E_m)t}\langle n|\rho(\mathbf{q},0)|m\rangle\langle m|\rho(-\mathbf{q},0)|n\rangle, \end{aligned} \tag{43}$$

where we have inserted a complete set $\sum_m |m\rangle\langle m|$, and used $e^{-iH_0 t}|m\rangle = e^{-iE_m t}|m\rangle$.

Since both $|n\rangle$ and $|m\rangle$ are manybody states of non-interacting particles, $\langle m|a_{ks}^\dagger a_{k-q,s}|n\rangle$ can be non-zero only if, when comparing to $|n\rangle$, the $|m\rangle$ state has one more electron at state $(\mathbf{k}, s)$, but one less electron at $(\mathbf{k}-\mathbf{q}, s)$. Therefore, $E_n - E_m = -\varepsilon_k + \varepsilon_{k-q}$, a difference of two single-particle energies. This energy factor can now be moved outside of the m-summation, and

$$\begin{aligned} & I(\mathbf{q};t,0) \\ = & \sum_n \frac{e^{-\beta E_n}}{Z}\sum_{k,s} e^{i(\varepsilon_{k-q}-\varepsilon_k)t}\langle n|a_{k-q,s}^\dagger a_{ks} a_{ks}^\dagger a_{k-q,s}|n\rangle \\ = & \sum_{k,s} e^{i(\varepsilon_{k-q}-\varepsilon_k)t}\sum_n \frac{e^{-\beta E_n}}{Z}\langle n|a_{k-q,s}^\dagger a_{k-q,s}(1-a_{ks}^\dagger a_{ks})|n\rangle \\ = & 2\sum_k e^{i(\varepsilon_{k-q}-\varepsilon_k)t} f(\varepsilon_{k-q})[1-f(\varepsilon_k)], \end{aligned} \tag{44}$$

where

$$f(\varepsilon_k) = \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|a_{ks}^\dagger a_{ks}|n\rangle \tag{45}$$

is the **Fermi distribution function** (spin-independent here). It is left as an exercise to show that

$$f(\varepsilon_k) = \frac{1}{1+e^{\beta\varepsilon_k}}. \tag{46}$$

Similarly, one can show that

$$I(-\mathbf{q};0,t) = 2\sum_k e^{i(\varepsilon_{k-q}-\varepsilon_k)t} f(\varepsilon_k)[1-f(\varepsilon_{k-q})]. \tag{47}$$

From Eq. (42), we have

$$\begin{aligned}\chi_\rho^0(\kappa) &= -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}[I(\mathbf{q};t,0)-I(-\mathbf{q};0,t)] \quad (48)\\ &= -\frac{2i}{V_0}\sum_k\int_0^\infty dt e^{i\omega t}e^{i(\varepsilon_{k-q}-\varepsilon_k)t}[f(\varepsilon_{k-q})-f(\varepsilon_k)].\end{aligned}$$

The integral over time is

$$\int_0^\infty dt e^{i(\omega+i\delta)t}e^{i(\varepsilon_{k-q}-\varepsilon_k)t} = \frac{i}{\omega+i\delta+(\varepsilon_{k-q}-\varepsilon_k)}. \tag{49}$$

The positive infinitesimal δ is added to ensure the convergence of the exponential at $t=\infty$.

Finally,

$$\chi_\rho^0(\mathbf{q},\omega) = \frac{2}{V_0}\sum_k\frac{f(\varepsilon_{k-q})-f(\varepsilon_k)}{\omega+i\delta+(\varepsilon_{k-q}-\varepsilon_k)}, \tag{50}$$

and

$$\epsilon(\mathbf{q},\omega) = 1-\frac{4\pi e^2}{q^2}\frac{2}{V_0}\sum_k\frac{f(\varepsilon_{k-q})-f(\varepsilon_k)}{\omega+i\delta+(\varepsilon_{k-q}-\varepsilon_k)}. \tag{51}$$

This is called the **Lindhard dielectric function**.

1. Low frequency limit

For frequency as low as $\omega \ll v_F q$, the ω in the denominator can be neglected, and

$$\chi_\rho^0(\mathbf{q},0) \simeq \frac{2}{V_0}\sum_k\frac{f(\varepsilon_{k-q})-f(\varepsilon_k)}{\varepsilon_{k-q}-\varepsilon_k}. \tag{52}$$

For general wave length (in 3-dim), it can be shown that

$$\chi_\rho^0(\mathbf{q},0) \simeq -D(\varepsilon_F)F\left(\frac{q}{2k_F}\right), \tag{53}$$

where $D(\varepsilon_F)$ is the density of states at the Fermi energy, and

$$F(x) = \frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| \tag{54}$$

is the Lindhard function (see Sec. II.A).

At long wavelength,

$$\chi_\rho^0(\mathbf{q},0) \simeq -\frac{2}{V_0}\sum_k\left(-\frac{\partial f_k}{\partial\varepsilon}\right) = -D(\varepsilon_F). \tag{55}$$

In this limit, the dielectric function is

$$\epsilon(\mathbf{q},0) = 1+\frac{k_{TF}^2}{q^2}, \tag{56}$$

where $k_{TF}^2 = 4\pi e^2 D(\varepsilon_F)$ is the **Thomas-Fermi wave vector**.

2. High frequency limit

The response function in Eq. (50) can be re-written as

$$\chi_\rho^0(\mathbf{q},\omega) = -\frac{2}{V_0}\sum_k f(\varepsilon_k)\frac{2(\varepsilon_{k-q}-\varepsilon_k)}{\omega^2-(\varepsilon_{k-q}-\varepsilon_k)^2}. \tag{57}$$

For high frequency and long wave length ($\omega \gg v_F q$),

$$\chi_\rho^0(0,\omega) \simeq \frac{q^2}{m\omega^2}\frac{2}{V_0}\sum_k f(\varepsilon_k) = \frac{q^2 n}{m\omega^2}, \tag{58}$$

where n is the particle density. Therefore,

$$\epsilon(0,\omega) = 1-\frac{\omega_p^2}{\omega^2}, \tag{59}$$

where $\omega_p^2 = 4\pi n e^2/m$ is the **plasma frequency**.

Notice that

$$\lim_{q\to 0}\lim_{\omega\to 0}\epsilon(\mathbf{q},\omega) \neq \lim_{\omega\to 0}\lim_{q\to 0}\epsilon(\mathbf{q},\omega). \tag{60}$$

That is, the dielectric function is not analytic at $(\mathbf{q},\omega) = (0,0)$.

III. CURRENT RESPONSE AND CONDUCTIVITY

In this section, we consider the generation of electron current caused by an external electric field. Before perturbation,

$$H_0 = \int dv \psi^\dagger(\mathbf{r})\frac{p^2}{2m}\psi(\mathbf{r})+V_L+V_{ee}, \tag{61}$$

where V_L is the one-body interaction, and V_{ee} is the electron interaction. In general, the external electric field depends on both scalar and vector potentials,

$$\mathbf{E}(\mathbf{r},t) = -\nabla\phi-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}. \tag{62}$$

For a static field, it is common to use $\mathbf{E} = -\nabla\phi$, as in Eq. (15). A static and uniform field then has $\phi(\mathbf{r}) = -\mathbf{E}\cdot\mathbf{r}$. A disadvantage of this scalar potential is that it is not bounded at infinity. To avoid such a problem, one can choose a gauge such that

$$\mathbf{E}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}. \tag{63}$$

In this case, a static and uniform field has $\mathbf{A}(t) = -c\mathbf{E}t$.

After applying the electric field, the Hamiltonian becomes

$$\begin{aligned}H &= \int dv \psi^\dagger(\mathbf{r})\frac{\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2}{2m}\psi(\mathbf{r})+V_L+V_{ee} \quad (64)\\ &= H_0+\frac{e}{2mc}\int dv\left(\psi^\dagger\mathbf{p}\cdot\mathbf{A}\psi+\psi^\dagger\mathbf{A}\cdot\mathbf{p}\psi\right)\\ &+ \frac{e^2}{2mc^2}\int dv A^2\psi^\dagger\psi,\end{aligned}$$

where H_0 refers to the parts that do not depend on $\mathbf{A}$. The particle current density operator $\mathbf{J}$ is related to the variation of the Hamiltonian as follows,

$$\delta H = \frac{e}{c}\int dv \mathbf{J}\cdot\delta\mathbf{A}, \tag{65}$$

where

$$\mathbf{J} \equiv \underbrace{\frac{1}{2mi}\left[\psi^\dagger\nabla\psi - \left(\nabla\psi^\dagger\right)\psi\right]}_{\text{paramagnetic current } \mathbf{J}^p} + \underbrace{\frac{e}{mc}\mathbf{A}\psi^\dagger\psi.}_{\text{diamagnetic current } \mathbf{J}^A} \tag{66}$$

We would like to find out the connection between $\langle\mathbf{J}\rangle$ and $\mathbf{A}$ (to first order). After perturbation, a manybody state

$$|n^0\rangle \to |n\rangle \simeq |n^0\rangle + |n^1\rangle, \tag{67}$$

where $|n^1\rangle$ is of order $\mathbf{A}$. Therefore,

$$\langle n|\mathbf{J}|n\rangle = \langle n^0|\mathbf{J}^A|n^0\rangle + \langle n^0|\mathbf{J}^p|n^1\rangle + \langle n^1|\mathbf{J}^p|n^0\rangle + O(A^2). \tag{68}$$

We have assumed, of course, that the equilibrium state carries no current, $\langle n^0|\mathbf{J}^p|n^0\rangle = 0$.

After taking the thermal average, the first term becomes

$$\langle\mathbf{J}^A\rangle = \frac{e}{mc}\mathbf{A}(\mathbf{r},t)\langle\rho(\mathbf{r})\rangle. \tag{69}$$

The other two terms are evaluated using the Kubo formula in Eq. (12), with the following replacement,

$$\begin{aligned} A &\to J^p_\alpha, \\ \mathbf{B} &\to \mathbf{J}^p, \\ \mathbf{f} &\to \frac{e}{c}\mathbf{A}. \end{aligned} \tag{70}$$

This gives us (recall that $x = (\mathbf{r},t)$)

$$\langle J^p_\alpha(x)\rangle = \frac{e}{c}\int dx' \chi^p_{\alpha\beta}(x,x')A_\beta(x'), \tag{71}$$

where

$$\chi^p_{\alpha\beta}(x,x') = -i\theta(t-t')\left\langle\left[J^p_\alpha(x), J^p_\beta(x')\right]\right\rangle. \tag{72}$$

After combining with the diamagnetic term in Eq. (69), the response function for the total current is

$$\chi_{\alpha\beta}(x,x') = \delta_{\alpha\beta}\delta(x-x')\frac{\rho(x)}{m} + \chi^p_{\alpha\beta}(x,x'). \tag{73}$$

Since H_0 is time independent, the response function $\chi_{\alpha\beta}(x,x') = \chi_{\alpha\beta}(\mathbf{r},\mathbf{r}';t-t')$. Applying the convolution theorem to the time variable (see Eq. (21)), one has

$$\langle J_\alpha(\mathbf{r},\omega)\rangle = \frac{e}{c}\int dv' \chi_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)A_\beta(\mathbf{r}',\omega). \tag{74}$$

The vector potential is related to the electric field as follows,

$$\mathbf{E}(\omega) = i\frac{\omega}{c}\mathbf{A}(\omega). \tag{75}$$

Therefore, for the electric current density $\mathbf{J}^e = -e\mathbf{J}$, one has

$$\langle J^e_\alpha(\mathbf{r},\omega)\rangle = \int dv' \sigma^p_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)E_\beta(\mathbf{r}',\omega). \tag{76}$$

The **conductivity tensor** is

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = i\frac{e^2}{\omega}\chi_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega). \tag{77}$$

Since the conductivity in general is a non-local quantity, the current density at point $\mathbf{r}$ would not only depend on the electric field at $\mathbf{r}$, but also on neighboring electric field.

For a homogeneous material,

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = \sigma_{\alpha\beta}(\mathbf{r}-\mathbf{r}';\omega). \tag{78}$$

We can then apply the convolution theorem to the space variable and get

$$\langle J^e_\alpha(\mathbf{q},\omega)\rangle = \sigma_{\alpha\beta}(\mathbf{q},\omega)E_\beta(\mathbf{q},\omega), \tag{79}$$

where

$$\sigma_{\alpha\beta}(\mathbf{q},\omega) = i\frac{e^2}{\omega}\left[\delta_{\alpha\beta}\frac{\rho(\mathbf{q},\omega)}{m} + \chi^p_{\alpha\beta}(\mathbf{q},\omega)\right], \tag{80}$$

in which (Cf. eq. (27))

$$\chi^p_{\alpha\beta}(\mathbf{q},\omega) = -\frac{i}{V_0}\int dt\theta(t-t')e^{i\omega(t-t')}\langle[J_\alpha(\mathbf{q},t), J_\beta(-\mathbf{q},t')]\rangle. \tag{81}$$

Notice that the diamagnetic part diverges as $\omega \to 0$. For usual conductors and insulators, this divergence would be cancelled by part of the paramagnetic term, so that the DC conductivity remains finite. In a superconductor (which is a perfect diamagnet), the paramagnetic term vanishes in the DC limit, and the conductivity is purely imaginary,

$$\sigma^{SC}_{\alpha\beta}(\mathbf{q},\omega) = i\frac{e^2}{\omega}\delta_{\alpha\beta}\frac{\rho(\mathbf{q},\omega)}{m}. \tag{82}$$

A purely imaginary conductivity leads to inductive behavior, and would not cause energy dissipation.

A. Conductivity for non-interacting electrons

We would like to start from a formulation that does not presume spacial homogeneity:

$$\chi^p_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}\langle\left[J^p_\alpha(\mathbf{r},t), J^p_\beta(\mathbf{r}',0)\right]\rangle, \tag{83}$$

where $J^p_\alpha(\mathbf{r},t) = e^{iH_0t}J^p_\alpha(\mathbf{r})e^{-iH_0t}$. Therefore,

$$\begin{aligned} & I_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',0) \\ \equiv & \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|J^p_\alpha(\mathbf{r},t)J^p_\beta(\mathbf{r}',0)|n\rangle \\ = & \sum_{n,m}\frac{e^{-\beta E_n}}{Z}e^{i(E_n-E_m)t}\langle n|J^p_\alpha(\mathbf{r},0)|m\rangle\langle m|J^p_\beta(\mathbf{r}',0)|n\rangle, \end{aligned} \tag{84}$$

in which we have inserted a complete set $\sum_m |m\rangle\langle m|$, and used $e^{-iH_0 t}|m\rangle = e^{-iE_m t}|m\rangle$ (see Sec. II.C).

The current density operator can be written as (see Chap 1)

$$J^p_\alpha(\mathbf{r}) = \sum_{\mu\nu}\langle\mu|J^{(1)}_\alpha(\mathbf{r})|\nu\rangle a^\dagger_\mu a_\nu, \tag{85}$$

where $J^{(1)}_\alpha$ is a one-body operator to be specified later.

From now on, assume the electrons are non-interacting. Substitute $J^p_\alpha(\mathbf{r})$ into Eq. (84), we get terms with the form

$$\langle n|a^\dagger_1 a_2|m\rangle\langle m|a^\dagger_3 a_4|n\rangle, \tag{86}$$

where $1, 2\cdots$ are simplified notations for single-particle state labels μ, ν. For this type of term to be non-zero, the single-particle states have to satisfy $(1 = 4, 2 = 3)$, or $(1 = 2, 3 = 4)$. They both lead to $E_n - E_m = \varepsilon_1 - \varepsilon_2$ (the second case has $\varepsilon_1 = \varepsilon_2$).

The summation over m can now be removed, and

$$\begin{aligned} I_{\alpha\beta}(\mathbf{r}, t, \mathbf{r}', 0) &= \sum_{1,2,3,4} e^{i(\varepsilon_1-\varepsilon_2)t}\langle 1|J^{(1)}_\alpha|2\rangle\langle 3|J^{(1)}_\beta|4\rangle \\ &\times \langle a^\dagger_1 a_2 a^\dagger_3 a_4\rangle(\delta_{14}\delta_{23} + \delta_{12}\delta_{34}). \end{aligned} \tag{87}$$

The thermal averages are (see Eq. (45))

$$\begin{aligned} \langle a^\dagger_1 a_2 a^\dagger_2 a_1\rangle &= f_1(1 - f_2), \\ \langle a^\dagger_1 a_1 a^\dagger_2 a_2\rangle &= f_1 f_2. \end{aligned} \tag{88}$$

where f is the Fermi distribution function. As a result, one can show that

$$\begin{aligned} &I_{\alpha\beta}(\mathbf{r}, t, \mathbf{r}', 0) - I_{\beta\alpha}(\mathbf{r}', 0, \mathbf{r}, t) \\ &= \sum_{12} e^{i(\varepsilon_1-\varepsilon_2)t}\langle 1|J^{(1)}_\alpha|2\rangle\langle 2|J^{(1)}_\beta|1\rangle(f_1 - f_2). \end{aligned} \tag{89}$$

Therefore,

$$\begin{aligned} &\chi^P_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega) \\ &= -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}[I_{\alpha\beta}(\mathbf{r}, t, \mathbf{r}', 0) - I_{\beta\alpha}(\mathbf{r}', 0, \mathbf{r}, t)] \\ &= \frac{1}{V_0}\sum_{12}(f_1 - f_2)\frac{\langle 1|J^{(1)}_\alpha(\mathbf{r})|2\rangle\langle 2|J^{(1)}_\beta(\mathbf{r}')|1\rangle}{\Omega + \varepsilon_1 - \varepsilon_2}, \end{aligned} \tag{90}$$

where $\Omega \equiv \omega + i\delta$

If the material is homogeneous, then

$$\chi^P_{\alpha\beta}(\mathbf{q}, \omega) = \frac{1}{V_0}\sum_{12}(f_1 - f_2)\frac{\langle 1|J^{(1)}_\alpha(\mathbf{q})|2\rangle\langle 2|J^{(1)}_\beta(-\mathbf{q})|1\rangle}{\Omega + \varepsilon_1 - \varepsilon_2}, \tag{91}$$

The one-body operator is (see Chap 1)

$$J^{(1)}_\alpha(\mathbf{q}) = \frac{1}{2m}\left(p_\alpha e^{-i\mathbf{q}\cdot\mathbf{r}} + e^{-i\mathbf{q}\cdot\mathbf{r}}p_\alpha\right) \tag{92}$$

1. Uniform limit

For the uniform case ($q = 0$), the conductivity is

$$\begin{aligned} &\sigma_{\alpha\beta}(0, \omega) \\ &= \frac{ie^2}{\omega}\left[\delta_{\alpha\beta}\frac{\rho(\omega)}{m} + \frac{1}{m^2 V_0}\sum_{\mu\nu}(f_\mu - f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\Omega + \varepsilon_\mu - \varepsilon_\nu}\right]. \end{aligned} \tag{93}$$

(We have re-written $1, 2$ as μ, ν.)

The denominator can be decomposed as

$$\frac{1}{\epsilon_{\mu\nu} \pm \Omega} = \frac{1}{\varepsilon_{\mu\nu}}\left(1 \mp \frac{\Omega}{\varepsilon_{\mu\nu} \pm \Omega}\right), \tag{94}$$

where $\varepsilon_{\mu\nu} \equiv \varepsilon_\mu - \varepsilon_\nu$. Substitute this to Eq. (93), then the first term of the decomposition would cancel with the diamagnetic term, because of the following **f-sum rule**:

$$\frac{1}{V_0}\sum_{\mu\nu}(f_\mu - f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\varepsilon_{\mu\nu}} = -m\rho\delta_{\alpha\beta}. \tag{95}$$

As a result,

$$\sigma_{\alpha\beta}(0, \omega) = \frac{e^2}{iV_0}\sum_{\mu\nu}(f_\mu - f_\nu)\frac{\langle\mu|v_\alpha|\nu\rangle\langle\nu|v_\beta|\mu\rangle}{\varepsilon_{\mu\nu}(\Omega + \varepsilon_{\mu\nu})}, \tag{96}$$

where $v_\alpha = p_\alpha/m$. This is sometimes called the **Kubo-Greenwood formula**.

2. Uniform and static, Hall conductivity

Finally, we would like to consider the DC Hall conductivity as an example. According to Eq. (96), it can be re-written as

$$\sigma^{DC}_{\alpha\neq\beta} = \frac{e^2}{iV_0}\sum_{\mu\nu}f_\mu\frac{\langle\mu|v_\alpha|\nu\rangle\langle\nu|v_\beta|\mu\rangle - \langle\mu|v_\beta|\nu\rangle\langle\nu|v_\alpha|\mu\rangle}{\varepsilon^2_{\mu\nu}}. \tag{97}$$

If the single-particle states are Bloch states ($\mu \to n\mathbf{k}$), $\langle r|n\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}u_{nk}(\mathbf{r})$, where $u_{nk}(\mathbf{r})$ is the cell-periodic function, then one can show that

$$\sigma^{DC}_{\alpha\neq\beta} = \frac{e^2}{V_0}\sum_{nk}f_{nk}\underbrace{\frac{1}{i}\left(\left\langle\frac{\partial u_{nk}}{\partial k_\alpha}|\frac{\partial u_{nk}}{\partial k_\beta}\right\rangle - \left\langle\frac{\partial u_{nk}}{\partial k_\beta}|\frac{\partial u_{nk}}{\partial k_\alpha}\right\rangle\right)}_{\text{Berry curvature } \Omega^\gamma_{nk}}, \tag{98}$$

where α, β, and γ are cyclic. We will call this as the **TKNdN formula** (see Ref. 4).

In 2-dim, for a filled band,

$$C^{(n)}_1 \equiv \frac{1}{2\pi}\int_{\text{filled BZ}} d^2k\Omega^z_{nk} \tag{99}$$

must be an integer (see Sec. II.B of Ref. 5). Therefore, the Hall conductivity from filled bands is quantized,

$$\sigma^{DC}_{xy} = \frac{e^2}{h}\sum_{\text{filled } n}C^{(n)}_1, \tag{100}$$

where we have put back the $\hbar$ explicitly. The quantized (topological) nature of such an integral is first pointed out by D.J. Thouless to explain the **quantum Hall effect**.

Prob. 1 Derive the f-sum rule,

$$\frac{1}{V_0}\sum_{\mu\nu}(f_\mu - f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\varepsilon_{\mu\nu}} = -m\rho\delta_{\alpha\beta}. \tag{101}$$

Prob. 2 Start from Eq. (97), derive the TKNdN formula in Eq. (98).

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