Chap 3 Linear response theory

Ming-Che Chang

Department of Physics, National Taiwan Normal University, Taipei, Taiwan

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I. GENERAL FORMULATION

A piece of matter would be polarized, or conduct current under an external electric field,

$$\mathbf{P} = \chi_e \mathbf{E}, \tag{1}$$
$$\mathbf{j} = \sigma \mathbf{E}. \tag{2}$$

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

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

$$\langle A \rangle_0 = \frac{1}{Z_0} \sum_{\{n\}} e^{-\beta E^0_{\{n\}}} \langle \{n\}^0 | A | \{n\}^0 \rangle. \tag{3}$$

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

$$\langle A \rangle = \frac{1}{Z_0} \sum_{\{n\}} e^{-\beta E^0_{\{n\}}} \langle \{n\} | A | \{n\} \rangle = \langle A \rangle_0 + \delta \langle A \rangle. \tag{4}$$

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

Note that in the equation above, we do not alter the thermal distribution. This is valid only if the perturbation is fast (compared to the time for reaching thermal equilibrium), such that the thermal distribution of the system are left unaltered. This is a tricky assumption and the resulting response is called **adiabatic response**. On the other hand, if the perturbation is slow so that the system can be in equilibrium with the reservoir, then the response is called **isothermal response**. For in-depth discussions, see Sec. 3.2.11 of Ref. 1, and Sec. 8.3 of Ref. 2.

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,

$$H_0 |n^0\rangle = E^0_n |n^0\rangle, \tag{5}$$

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

$$H(t) = H_0 + H'(t). \tag{6}$$

After the perturbation ($\hbar \equiv 1$),

$$H(t)|n(t)\rangle = i\frac{\partial}{\partial t}|n(t)\rangle. \tag{7}$$

It is helpful to write,

$$|n(t)\rangle = e^{-iH_0 t}|n_I(t)\rangle. \tag{8}$$

Then,

$$H'_I(t)|n_I(t)\rangle = i\frac{\partial}{\partial t}|n_I(t)\rangle. \tag{9}$$

where

$$H'_I(t) \equiv e^{iH_0 t} H' e^{-iH_0 t}, \tag{10}$$

We say that the states and operators with subscript I are in the **interaction picture**.

To linear order,

$$|n_I(t)\rangle \simeq |n^0_I\rangle - i\int_{-\infty}^t dt' H'_I(t')|n^0_I\rangle. \tag{11}$$

Substitute it into Eq. (4), and keep only the terms to linear order in H'_I, we have

$$\begin{aligned} &\langle A(t)\rangle \\ &= \langle A\rangle_0 - i\int_{-\infty}^t dt' \sum_n \langle n^0|[A_I(t), H'_I(t')]|n^0\rangle \frac{e^{-\beta E^0_n}}{Z_0} \\ &= \langle A\rangle_0 - i\int_{-\infty}^t dt' \langle [A_I(t), H'_I(t')]\rangle_0, \end{aligned} \tag{12}$$

where

$$A_I(t) \equiv e^{iH_0 t} A e^{-iH_0 t}. \tag{13}$$

For example, if the following perturbation is turned on abruptly at t_0,

$$H'(t) = \int dv \underbrace{\mathbf{B}(\mathbf{r})}_{\text{operator}} \cdot \underbrace{\mathbf{f}(\mathbf{r},t)}_{C-\text{number}}, \tag{14}$$

then

$$\begin{aligned} &\delta\langle A(\mathbf{r},t)\rangle \\ &= -i\int dv' \int_{t_0}^t dt' \langle [A_I(\mathbf{r},t), \mathbf{B}_I(\mathbf{r}',t')]\rangle_0 \cdot \mathbf{f}(\mathbf{r}',t') \\ &= -i\int dv' \int_{t_0}^\infty dt' \theta(t-t') \langle [A_I(\mathbf{r},t), \mathbf{B}_I(\mathbf{r}',t')]\rangle_0 \cdot \mathbf{f}(\mathbf{r}',t'). \end{aligned} \tag{15}$$

This can be written as

$$\delta\langle A(x)\rangle = \int dx' \sum_\alpha \chi_{AB_\alpha}(x,x') f_\alpha(x'), \tag{16}$$

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

$$\chi_{AB_\alpha}(x, x') = -i\theta(t-t')\langle[A_I(x), B_{I\alpha}(x')]\rangle_0. \quad (17)$$

We will eventually let $t_0 \to -\infty$, so that both space and time integrals cover the whole space-time. Eq (16) is called the **Kubo formula**, and χ_{AB_α} is called the **response function**. Be aware 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,

$$H_0 = T + V_L + V_{ee}, \quad (18)$$

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,

$$H' = \int dv \rho_e(\mathbf{r})\phi_{ext}(\mathbf{r}, t), \quad (19)$$

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

Because of the external potential, electron density

$$\langle\rho_e\rangle_0 \to \langle\rho_e\rangle = \langle\rho_e\rangle_0 + \delta\langle\rho_e\rangle. \quad (20)$$

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

$$\begin{aligned} A &\to \rho_e, & (21)\\ \mathbf{B} &\to \rho_e, & (22)\\ \mathbf{f} &\to \phi_{ext}. & (23) \end{aligned}$$

The Kubo formula gives

$$\delta\langle\rho_e(x)\rangle = \int dx' \chi_{\rho_e}(x, x')\phi_{ext}(x'), \quad (24)$$

and the response function is

$$\chi_{\rho_e}(x, x') = -i\theta(t-t')\langle[\rho_e(x), \rho_e(x')]\rangle_0. \quad (25)$$

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

$$\chi_{\rho_e}(x, x') = \chi_{\rho_e}(x - x'). \quad (26)$$

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

$$\delta\langle\rho_e(\kappa)\rangle = \chi_{\rho_e}(\kappa)\phi_{ext}(\kappa), \quad (27)$$

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

$$\begin{aligned} \delta\langle\rho_e(x)\rangle &= \sum_\kappa e^{i\kappa x}\delta\langle\rho_e(\kappa)\rangle, & (28)\\ \delta\langle\rho_e(\kappa)\rangle &= \int dx e^{-i\kappa x}\delta\langle\rho_e(x)\rangle; & (29)\\ \phi_{ext}(x) &= \sum_\kappa e^{i\kappa x}\phi_{ext}(\kappa), & (30)\\ \phi_{ext}(\kappa) &= \int dx e^{-i\kappa x}\phi_{ext}(x). & (31) \end{aligned}$$

The summation over κ should be understood as

$$\sum_\kappa = \frac{1}{V_0}\sum_{\mathbf{q}}\int\frac{d\omega}{2\pi}. \quad (32)$$

The Fourier expansion of the response function is

$$\chi_{\rho_e}(x - x') \equiv \sum_\kappa e^{i\kappa(x-x')}\chi_{\rho_e}(\kappa), \quad (33)$$

and

$$\begin{aligned} \chi_{\rho_e}(\kappa) &= \int d(x-x')e^{-i\kappa(x-x')}\chi_{\rho_e}(x-x')\\ &= -i\int d(t-t')\theta(t-t')e^{i\omega(t-t')} \quad (34)\\ &\times \int d^3(\mathbf{r}-\mathbf{r}')e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\langle[\rho_e(\mathbf{r}, t), \rho_e(\mathbf{r}', t')]\rangle_0. \end{aligned}$$

Since the system is uniform in space, one can perform an extra space integral $\frac{1}{V_0}\int d^3\mathbf{r}'$ to the space integral above, and use

$$\frac{1}{V_0}\int d^3\mathbf{r}'\int d^3(\mathbf{r}-\mathbf{r}') = \frac{1}{V_0}\int d^3\mathbf{r}\int d^3\mathbf{r}'. \quad (35)$$

Then it is not difficult to see that

$$\chi_{\rho_e}(\kappa) = -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}\langle[\rho_e(\mathbf{q}, t), \rho_e(-\mathbf{q}, 0)]\rangle_0. \quad (36)$$

Note 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

$$\begin{aligned} \rho_e &= -e\rho, \quad \chi_{\rho_e} = e^2\chi_\rho, & (37)\\ \text{and}\ \delta\langle\rho\rangle &= -e\chi_\rho\phi_{ext}. & (38) \end{aligned}$$

Also, note that these response functions are related to, but not the same as, the electric susceptibility χ_e mentioned 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,

$$\phi(\kappa) = \phi_{ext}(\kappa) + \delta\phi(\kappa), \quad (39)$$

and

$$\epsilon(\kappa) = \frac{\phi_{ext}(\kappa)}{\phi(\kappa)}. \tag{40}$$

The total particle density is

$$\langle\rho\rangle = \langle\rho\rangle_{ext} + \delta\langle\rho\rangle. \tag{41}$$

Particle densities are related to the potentials via the Poisson equations,

$$q^2\phi_{ext}(\kappa) = -4\pi e\langle\rho(\kappa)\rangle_{ext}, \tag{42}$$
$$q^2\phi(\kappa) = -4\pi e\langle\rho(\kappa)\rangle. \tag{43}$$

Note that quantities such as $\phi_{ext}(\kappa) = \phi_{ext}(\mathbf{q},\omega)$ is allowed to be frequency-dependent. If SI is used, then just replace 4π with $\frac{1}{\epsilon_0}$.

Combine the three equations above, we get a relation between ϕ and ϕ_{ext},

$$\phi(\kappa) = \phi_{ext} + 4\pi e^2\chi_\rho\frac{\phi_{ext}}{q^2}. \tag{44}$$

This leads to a relation between ϵ and χ_ρ,

$$\frac{1}{\epsilon(\kappa)} = 1 + \underbrace{\frac{4\pi e^2}{q^2}}_{V^{(2)}(\mathbf{q})}\chi_\rho, \tag{45}$$

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

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

$$\delta\langle\rho\rangle = -e\chi_\rho^0\phi, \quad \phi = \phi_{ext} + \delta\phi. \tag{46}$$

It's not difficult to see that,

$$\chi_\rho = \frac{\chi_\rho^0}{1 - \frac{4\pi e^2}{q^2}\chi_\rho^0}, \tag{47}$$

and

$$\epsilon(\kappa) = 1 - \frac{4\pi e^2}{q^2}\chi_\rho^0. \tag{48}$$

Thus, given $\phi_{ext} = 4\pi e^2/q^2 \equiv V(q)$, one has

$$V_{eff}(q) = \frac{V(q)}{\epsilon(q)} = \frac{V(q)}{1 - V(q)\chi_\rho^0(q)}. \tag{49}$$

The calculation of χ_ρ is based on Eq. (36), 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 (Ref. 3):

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

$$V_{ee} = \frac{1}{2}\int dvdv'V^{(2)}(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r})\rho_e(\mathbf{r}'). \tag{50}$$

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

$$\rho_e(\mathbf{r}) = \langle\rho_e(\mathbf{r})\rangle + \underbrace{\rho_e(\mathbf{r}) - \langle\rho_e(\mathbf{r})\rangle}_{\delta\rho_e(\mathbf{r})}. \tag{51}$$

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

$$\begin{aligned} V_{ee} &\simeq \int dvdv'V^{(2)}(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r})\langle\rho_e(\mathbf{r}')\rangle \\ &- \frac{1}{2}\int dvdv'V^{(2)}(\mathbf{r}-\mathbf{r}')\langle\rho_e(\mathbf{r})\rangle\langle\rho_e(\mathbf{r}')\rangle. \end{aligned} \tag{52}$$

The mean-field Hamiltonian under perturbation is (dropping the second term in Eq. (52)),

$$\begin{aligned} &H_{MF} \\ &= \tilde{H}_0 + \int dvdv'V^{(2)}(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r})\langle\rho_e(\mathbf{r}')\rangle + \int dv\rho_e(\mathbf{r})\phi_{ext} \\ &= \tilde{H}_0 + \int dv\rho_e(\mathbf{r})\phi(\mathbf{r}), \end{aligned} \tag{53}$$

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

$$\phi(\mathbf{r}) = \phi_{ext}(\mathbf{r}) + \int dv'V^{(2)}(\mathbf{r}-\mathbf{r}')\langle\rho_e(\mathbf{r}')\rangle. \tag{54}$$

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

$$\chi_\rho^0(\kappa) = -\frac{i}{V_0}\int_0^\infty dte^{i\omega t}\langle[\rho(\mathbf{q},t),\rho(-\mathbf{q},0)]\rangle. \tag{55}$$

In the interaction picture, $\rho(\mathbf{q},t) = e^{iH_0t}\rho(\mathbf{q})e^{-iH_0t}$. The summation

$$\begin{aligned} &I(\mathbf{q};t,0) \\ &\equiv \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|\rho(\mathbf{q},t)\rho(-\mathbf{q},0)|n\rangle \\ &= \sum_{n,m}\frac{e^{-\beta E_n}}{Z}e^{i(E_n-E_m)t}\langle n|\rho(\mathbf{q},0)|m\rangle\langle m|\rho(-\mathbf{q},0)|n\rangle, \end{aligned} \tag{56}$$

where we have inserted a complete set $\sum_m |m\rangle\langle m|$, and used $e^{-iH_0t}|m\rangle = e^{-iE_mt}|m\rangle$.

Since both $|n\rangle$ and $|m\rangle$ are manybody states of non-interacting particles, $\langle m|a^\dagger_{ks}a_{k-q,s}|n\rangle$ can be non-zero only if, when comparing with $|n\rangle$, 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. It follows that,

$$\begin{aligned} & I(\mathbf{q};t,0) \\ = & \sum_n \frac{e^{-\beta E_n}}{Z} \sum_{k,s} e^{i(\varepsilon_{k-q}-\varepsilon_k)t} \langle n|a^\dagger_{k-q,s}a_{ks}a^\dagger_{ks}a_{k-q,s}|n\rangle. \end{aligned} \tag{57}$$

For free-particle or Hartree-Fock-like states (consider $q \neq 0$),

$$\langle a^\dagger_{k-q,s}a_{ks}a^\dagger_{ks}a_{k-q,s}\rangle = \langle a^\dagger_{k-q,s}a_{k-q,s}\rangle\langle a_{ks}a^\dagger_{ks}\rangle. \tag{58}$$

This is related to the **Wick theorem** at finite temperature. See, e.g., Appendix 3 of Ref. 1 and related discussion. The $q = 0$ term, if not dropped, would be cancelled out in Eq. (63) below anyway. Now, it is left as an exercise to show that,

$$\begin{aligned} f(\varepsilon_k) \equiv \langle a^\dagger_{ks}a_{ks}\rangle &= \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|a^\dagger_{ks}a_{ks}|n\rangle \\ &= \frac{1}{1+e^{\beta\varepsilon_k}}. \end{aligned} \tag{59}$$

Thus,

$$I(\mathbf{q};t,0) = 2\sum_k e^{i(\varepsilon_{k-q}-\varepsilon_k)t} f(\varepsilon_{k-q})[1-f(\varepsilon_k)]. \tag{60}$$

Had grand canonical ensemble been used, we'd have

$$f(\varepsilon_k) = \frac{1}{1+e^{\beta(\varepsilon_k-\mu)}}. \tag{61}$$

This is the **Fermi-Dirac distribution function** (spin-independent here).

Similarly, one can show that,

$$I(-\mathbf{q};0,t) = 2\sum_k e^{i(\varepsilon_{k-q}-\varepsilon_k)t} f(\varepsilon_k)[1-f(\varepsilon_{k-q})]. \tag{62}$$

From Eq. (55), we have

$$\begin{aligned} \chi^0_\rho(\kappa) &= -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}[I(\mathbf{q};t,0) - I(-\mathbf{q};0,t)] \qquad (63) \\ &= -\frac{2i}{V_0}\sum_k \int_0^\infty dt e^{i\omega t} e^{i(\varepsilon_{k-q}-\varepsilon_k)t}[f(\varepsilon_{k-q}) - f(\varepsilon_k)]. \end{aligned}$$

The integral over time is

$$\int_0^\infty dt e^{i(\omega+i\delta)t} e^{i(\varepsilon_{k-q}-\varepsilon_k)t} = \frac{i}{\omega + i\delta + (\varepsilon_{k-q}-\varepsilon_k)}. \tag{64}$$

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

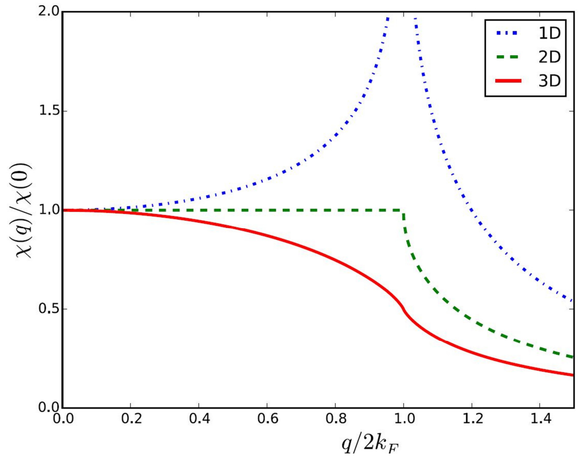

FIG. 1 Electric susceptibility of electron gas in different dimensions. Fig from Dugdale's Phys Scr, 2016.

Finally,

$$\chi^0_\rho(\mathbf{q},\omega) = \frac{2}{V_0}\sum_k \frac{f(\varepsilon_{k-q}) - f(\varepsilon_k)}{\omega + i\delta + (\varepsilon_{k-q}-\varepsilon_k)}, \tag{65}$$

and

$$\epsilon(\mathbf{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\frac{2}{V_0}\sum_k \frac{f(\varepsilon_{k-q}) - f(\varepsilon_k)}{\omega + i\delta + (\varepsilon_{k-q}-\varepsilon_k)}. \tag{66}$$

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

$$\chi^0_\rho(\mathbf{q},0) \simeq \frac{2}{V_0}\sum_k \frac{f(\varepsilon_{k-q}) - f(\varepsilon_k)}{\varepsilon_{k-q}-\varepsilon_k}. \tag{67}$$

Recall that we are calculating the adiabatic response (see Sec. I), which presumes the perturbation to be fast. Thus, it seems risky to apply our result to the low-frequency limit. However, for the density response, the result reported below is indeed valid. See p. 136 of Ref. 1 for an explanation.

At long wavelength,

$$\chi^0_\rho(\mathbf{q},0) \simeq -\frac{2}{V_0}\sum_k\left(-\frac{\partial f_k}{\partial\varepsilon}\right) = -D(\varepsilon_F), \tag{68}$$

where $D(\varepsilon_F)$ is the density of states at the Fermi energy. For 3D free electron gas,

$$D(\varepsilon_F) = \frac{mk_F}{\pi^2\hbar^2}. \tag{69}$$

In this limit, the dielectric function is

$$\epsilon(\mathbf{q},0) = 1 + \frac{k^2_{TF}}{q^2}, \tag{70}$$

where $k_{TF}^2 = 4\pi e^2 D(\varepsilon_F)$ is the **Thomas-Fermi wave vector**. For Copper, $k_{TF} \simeq 1.8 \times 10^{10}$/m. Thus the screening length $1/k_{TF} \simeq 0.55\AA$.

Given a point charge with $\phi_{ext}(\mathbf{r}) = Q/r$, the screened electrostatic potential is,

$$\begin{aligned}\phi(\mathbf{r}) &= \int \frac{d^3q}{(2\pi)^3}\frac{\phi_{ext}(\mathbf{q})}{\epsilon(\mathbf{q},0)}e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \int \frac{d^3q}{(2\pi)^3}\frac{4\pi Q}{q^2+k_{TF}^2}e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \frac{Q}{r}e^{-k_{TF}r}. \end{aligned} \tag{71}$$

For general wavelength (in 3D), it can be shown that (see Sec. 14 of Ref. 4),

$$\chi_\rho^0(\mathbf{q},0) \simeq -D(\varepsilon_F)F\left(\frac{q}{2k_F}\right), \tag{72}$$

where

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| \tag{73}$$

is the Lindhard function (see Sec. III.A). The slope of $F(q/2k_F)$ has a logarithmic singularity at $q = 2k_F$ (see Fig. 1), resulting in a sudden decrease of screening. This is related the fact that the pair creation energy, $\delta\varepsilon_q = \varepsilon_{k+q} - \varepsilon_k = \frac{\hbar^2}{m}q(\pm k_F + q/2)$, can no longer be zero once $q > 2k_F$ (see Fig. 3(a)).

It can be shown that (not easy), if we use Eq. (72), then for $k_F r \gg 1$, the induced charge density is (see Fig. 2),

$$\delta\rho(\mathbf{r}) \simeq \frac{\cos(2k_F r)}{r^3}. \tag{74}$$

One can see p. 178 of Ref. 4 for a derivation. The oscillation of $\delta\rho$ (and accompanied potential variation) is called the **Friedel oscillation**.

For reference, we show the electric susceptibility for electron gas in lower dimensions (see Fig. 1). In 2D, it is,

$$\chi_\rho^0(\mathbf{q}) = \begin{cases} -\frac{m}{\pi\hbar^2} & \text{if } q \le 2k_F, \\ -\frac{m}{\pi\hbar^2}\left[1-\sqrt{1-(2k_F/q)^2}\right] & \text{if } q > 2k_F. \end{cases} \tag{75}$$

In 1D, it is,

$$\chi_\rho^0(\mathbf{q}) = -\frac{2m}{\pi\hbar^2}\frac{1}{q}\ln\left(\frac{q+2k_F}{q-2k_F}\right), \tag{76}$$

which diverges at $q = 2k_F$. One can find more details in, e.g., Sec. 4.4 of Ref. 1.

2. High-frequency limit

The response function in Eq. (65) can be rewritten as,

$$\chi_\rho^0(\mathbf{q},\omega) = \frac{2}{V_0}\sum_k f(\varepsilon_k)\frac{2(\varepsilon_{k-q}-\varepsilon_k)}{\omega^2-(\varepsilon_{k-q}-\varepsilon_k)^2}. \tag{77}$$

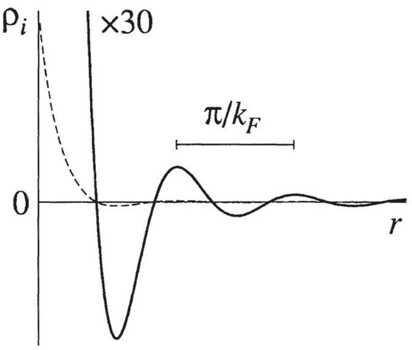

FIG. 2 Friedel oscillation. Fig from Chazalviel's *Coulomb screening by mobile charges.*

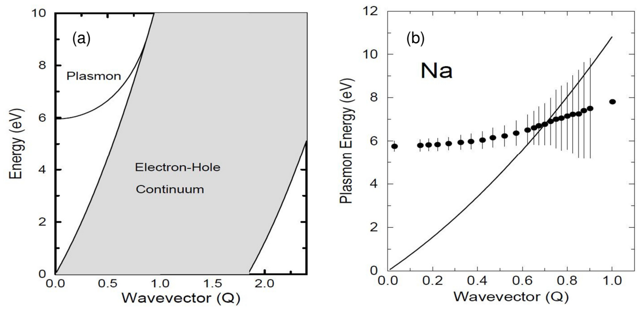

FIG. 3 (a) Predicted dispersion curve of the plasmon (in sodium) vs electron-hole continuum. (b) Measured plasmon dispersion in sodium. The vertical bars are measured widths of the plasmon resonances. Figs are from Ref. 5.

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

$$\chi_\rho^0(0,\omega) \simeq \frac{q^2}{m\omega^2}\frac{2}{V_0}\sum_k f(\varepsilon_k) = \frac{q^2 n}{m\omega^2}, \tag{78}$$

where n is the particle density. Therefore,

$$\epsilon(0,\omega) = 1 - \frac{\omega_p^2}{\omega^2}, \tag{79}$$

where $\omega_p^2 = 4\pi ne^2/m$ is the **plasma frequency**. For copper, $n = 8 \times 10^{22}/\text{cm}^3$, and the plasma frequency is $\omega_p = 1.6 \times 10^{16}$/s (corresponding to a wavelength about 1200 Å). A piece of metal becomes transparent to an EM wave with frequency ω if $\omega > \omega_p$.

It is possible to consider the shift of plasma frequency when q is finite. To leading order, we have

$$\epsilon(\mathbf{q},\omega) \simeq 1 - \frac{4\pi e^2}{m\omega^2}\frac{2}{V_0}\sum_k f(\varepsilon_k)\left(1+\frac{\hbar^2q^2}{m^2\omega^2}k^2\right). \tag{80}$$

At $T = 0$,

$$\frac{2}{V_0}\sum_k f(\varepsilon_k)k^2 = \frac{3}{5}nk_F^2. \tag{81}$$

It follows that,

$$\epsilon(\mathbf{q},\omega) \simeq 1 - \frac{\omega_p^2}{\omega^2}\left[1+\frac{3}{5}\left(\frac{\hbar k_F}{m\omega}\right)^2 q^2\right]. \tag{82}$$

There is longitudinal plasma oscillation when $\epsilon(\mathbf{q},\omega)=0$. Thus,

$$\omega^2=\omega_p^2+\frac{3}{5}v_F^2q^2+\cdots. \tag{83}$$

See Fig. 3 for details. The **electron-hole continuum** in Fig. 3(a) is the domain where the creation of an electron-hole pair out of a Fermi sphere is allowed (more in Chap 6).

For reference, the plasma frequency for 2D electron gas is,

$$\omega^2=\frac{2\pi ne^2}{m}q+\frac{3}{4}v_F^2q^2+\cdots, \tag{84}$$

which is *gapless*. See p. 204 of Ref. 1 for more details.

Finally, note that (see Eqs. (70), (79))

$$\lim_{q\to 0}\lim_{\omega\to 0}\epsilon(\mathbf{q},\omega)\neq\lim_{\omega\to 0}\lim_{q\to 0}\epsilon(\mathbf{q},\omega). \tag{85}$$

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

III. CURRENT RESPONSE AND CONDUCTIVITY

A. Current response

In this section, we consider the electric current driven by an external electric field. Before perturbation,

$$H_0=\int dv\psi^\dagger(\mathbf{r})\frac{p^2}{2m}\psi(\mathbf{r})+V_L+V_{ee}, \tag{86}$$

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

$$\mathbf{E}(\mathbf{r},t)=-\nabla\phi-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}. \tag{87}$$

For a static field, it is common to use $\mathbf{E}=-\nabla\phi$, as in Eq. (19). A static and uniform field then has $\phi(\mathbf{r})=-\mathbf{E}\cdot\mathbf{r}$, $\mathbf{A}(\mathbf{r})=0$. 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

$$\mathbf{E}(\mathbf{r},t)=-\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}. \tag{88}$$

In this case, a static and uniform field has $\mathbf{A}(t)=-c\mathbf{E}t$, and $\phi(\mathbf{r})=0$.

After applying the electric field, the Hamiltonian becomes,

$$\begin{aligned}H&=\int dv\psi^\dagger(\mathbf{r})\frac{\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2}{2m}\psi(\mathbf{r})+V_L+V_{ee}\\&=H_0+\frac{e}{2mc}\int dv\left(\psi^\dagger\mathbf{p}\cdot\mathbf{A}\psi+\psi^\dagger\mathbf{A}\cdot\mathbf{p}\psi\right)\\&+\frac{e^2}{2mc^2}\int dvA^2\psi^\dagger\psi,\end{aligned} \tag{89}$$

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,

$$\delta H=\frac{e}{c}\int dv\mathbf{J}\cdot\delta\mathbf{A}, \tag{90}$$

where

$$\mathbf{J}\equiv\underbrace{\frac{1}{2mi}\left[\psi^\dagger\nabla\psi-\left(\nabla\psi^\dagger\right)\psi\right]}_{\text{paramagnetic current }\mathbf{J}^p}+\underbrace{\frac{e}{mc}\mathbf{A}\psi^\dagger\psi.}_{\text{diamagnetic current }\mathbf{J}^A} \tag{91}$$

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

$$|n^0\rangle\to|n\rangle\simeq|n^0\rangle+|n^1\rangle, \tag{92}$$

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

$$\langle n|\mathbf{J}|n\rangle=\langle n^0|\mathbf{J}^A|n^0\rangle+\langle n^0|\mathbf{J}^p|n^1\rangle+\langle n^1|\mathbf{J}^p|n^0\rangle+O(A^2). \tag{93}$$

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,

$$\langle\mathbf{J}^A\rangle=\frac{e}{mc}\mathbf{A}(\mathbf{r},t)\rho(\mathbf{r}). \tag{94}$$

The other two terms are evaluated using the Kubo formula in Eq. (16), with the following replacement,

$$\begin{aligned}A&\to J^p_\alpha, &(95)\\ \mathbf{B}&\to\mathbf{J}^p, &(96)\\ \mathbf{f}&\to\frac{e}{c}\mathbf{A}. &(97)\end{aligned}$$

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

$$\langle J^p_\alpha(x)\rangle=\frac{e}{c}\int dx'\chi^p_{\alpha\beta}(x,x')A_\beta(x'), \tag{98}$$

where

$$\chi^p_{\alpha\beta}(x,x')=-i\theta(t-t')\left\langle\left[J^p_\alpha(x),J^p_\beta(x')\right]\right\rangle. \tag{99}$$

After combining with the diamagnetic term in Eq. (94), the response function for the total current is,

$$\chi_{\alpha\beta}(x,x')=\delta_{\alpha\beta}\delta(x-x')\frac{\rho(x)}{m}+\chi^p_{\alpha\beta}(x,x'). \tag{100}$$

Since H_0 is time independent, $\rho(x)=\rho(\mathbf{r})$, and 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. (27)), one has

$$\langle J_\alpha(\mathbf{r},\omega)\rangle=\frac{e}{c}\int dv'\chi_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)A_\beta(\mathbf{r}',\omega), \tag{101}$$

where

$$\chi_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = \delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{r}')\frac{\rho(\mathbf{r})}{m} + \chi^p_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega), \quad (102)$$

in which

$$\chi^p_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = -i\int dt\theta(t)e^{i\omega t}\langle[J_\alpha(\mathbf{r},t), J_\beta(\mathbf{r}',0)]\rangle. \quad (103)$$

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

$$\mathbf{E}(\omega) = i\frac{\omega}{c}\mathbf{A}(\omega). \quad (104)$$

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

$$\langle J^e_\alpha(\mathbf{r},\omega)\rangle = \int dv'\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)E_\beta(\mathbf{r}',\omega). \quad (105)$$

The **conductivity tensor** is

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = i\frac{e^2}{\omega}\chi_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega). \quad (106)$$

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,

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = \sigma_{\alpha\beta}(\mathbf{r}-\mathbf{r}';\omega). \quad (107)$$

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

$$\langle J^e_\alpha(\mathbf{q},\omega)\rangle = \sigma_{\alpha\beta}(\mathbf{q},\omega)E_\beta(\mathbf{q},\omega), \quad (108)$$

where

$$\sigma_{\alpha\beta}(\mathbf{q},\omega) = i\frac{e^2}{\omega}\left[\delta_{\alpha\beta}\frac{\rho_0}{m} + \chi^p_{\alpha\beta}(\mathbf{q},\omega)\right], \quad (109)$$

in which ρ_0 is the homogeneous particle density, and (Cf. Eq. (36))

$$\chi^p_{\alpha\beta}(\mathbf{q},\omega) = -\frac{i}{V_0}\int dt\theta(t)e^{i\omega t}\langle[J_\alpha(\mathbf{q},t), J_\beta(-\mathbf{q},0)]\rangle. \quad (110)$$

Note 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 (think of the Meissner effect), the paramagnetic term vanishes in the DC limit, and the conductivity is purely imaginary,

$$\sigma^{SC}_{\alpha\beta}(\mathbf{q},\omega) = i\frac{e^2}{\omega}\delta_{\alpha\beta}\frac{\rho_0}{m}. \quad (111)$$

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

B. Electrical conductivity

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

$$\chi^p_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) = -i\int_0^\infty dte^{i\omega t}\left\langle\left[J^p_\alpha(\mathbf{r},t), J^p_\beta(\mathbf{r}',0)\right]\right\rangle, \quad (112)$$

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

$$\begin{aligned} & I_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',0) \\ \equiv & \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|J^p_\alpha(\mathbf{r},t)J^p_\beta(\mathbf{r}',0)|n\rangle \quad (113) \\ = & \sum_{n,m}\frac{e^{-\beta E_n}}{Z}e^{i(E_n-E_m)t}\langle n|J^p_\alpha(\mathbf{r},0)|m\rangle\langle m|J^p_\beta(\mathbf{r}',0)|n\rangle. \end{aligned}$$

We have inserted a complete set $\sum_m |m\rangle\langle m|$, and used $e^{-iH_0t}|m\rangle = e^{-iE_mt}|m\rangle$.

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

$$J^p_\alpha(\mathbf{r}) = \sum_{\mu\nu}\langle\mu|J^{(1)}_\alpha(\mathbf{r})|\nu\rangle a^\dagger_\mu a_\nu, \quad (114)$$

where $J^{(1)}_\alpha(\mathbf{r})$ is the one-body operator that can be found in the Table of Chap 1.

From now on, assume the electrons are not interacting with each other. Substitute $J^p_\alpha(\mathbf{r})$ into Eq. (113), we get terms with the form,

$$\langle n|a^\dagger_1a_2|m\rangle\langle m|a^\dagger_3a_4|n\rangle, \quad (115)$$

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

$$\begin{aligned} I_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',0) &= \sum_{1,2,3,4} e^{i(\varepsilon_1-\varepsilon_2)t}\langle 1|J^{(1)}_\alpha|2\rangle\langle 3|J^{(1)}_\beta|4\rangle \\ &\times \langle a^\dagger_1a_2a^\dagger_3a_4\rangle(\delta_{14}\delta_{23}+\delta_{12}\delta_{34}). \quad (116) \end{aligned}$$

The thermal averages are (see Eq. (59)),

$$\langle a^\dagger_1a_2a^\dagger_2a_1\rangle = f_1(1-f_2), \quad (117)$$

$$\langle a^\dagger_1a_1a^\dagger_2a_2\rangle = f_1f_2. \quad (118)$$

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

$$\begin{aligned} & I_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',0) - I_{\beta\alpha}(\mathbf{r}',0,\mathbf{r},t) \\ = & \sum_{12} e^{i(\varepsilon_1-\varepsilon_2)t}\langle 1|J^{(1)}_\alpha|2\rangle\langle 2|J^{(1)}_\beta|1\rangle(f_1-f_2). \quad (119) \end{aligned}$$

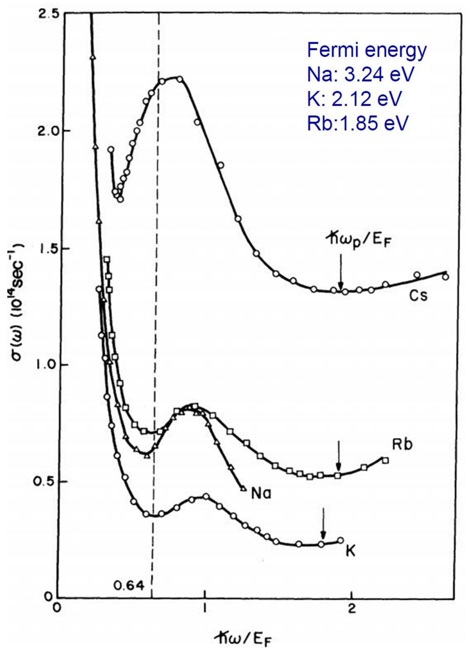

FIG. 4 Real part of the optical conductivity for alkali metals. The Drude peaks can be seen at low frequency. Smith, Phys Rev B **2**, 2840 (1970).

Therefore,

$$\begin{aligned}
&\chi^P_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) \\
&= -i\int_0^\infty dt e^{i\omega t}[I_{\alpha\beta}(\mathbf{r},t,\mathbf{r}',0) - I_{\beta\alpha}(\mathbf{r}',0,\mathbf{r},t)] \\
&= \sum_{12}(f_1 - f_2)\frac{\langle 1|J^{(1)}_\alpha(\mathbf{r})|2\rangle\langle 2|J^{(1)}_\beta(\mathbf{r}')|1\rangle}{\Omega+\varepsilon_1-\varepsilon_2}, \qquad (120)
\end{aligned}$$

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

If the material is homogeneous, then

$$\chi^P_{\alpha\beta}(\mathbf{q},\omega) = \frac{1}{V_0}\sum_{12}(f_1-f_2)\frac{\langle 1|J^{(1)}_\alpha(\mathbf{q})|2\rangle\langle 2|J^{(1)}_\beta(-\mathbf{q})|1\rangle}{\Omega+\varepsilon_1-\varepsilon_2}, \qquad (121)$$

in which (see Chap 1),

$$J^{(1)}_\alpha(\mathbf{q}) = \frac{1}{2m}\left(p_\alpha e^{-i\mathbf{q}\cdot\mathbf{r}} + e^{-i\mathbf{q}\cdot\mathbf{r}}p_\alpha\right). \qquad (122)$$

1. Uniform limit

For the uniform case ($q = 0$), the conductivity is (rewrite $1,2$ as μ,ν),

$$\begin{aligned}
&\sigma_{\alpha\beta}(0,\omega) \qquad (123)\\
&= \frac{ie^2}{\omega}\left[\delta_{\alpha\beta}\frac{\rho_0}{m} + \frac{1}{m^2V_0}\sum_{\mu\nu}(f_\mu-f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\Omega+\varepsilon_\mu-\varepsilon_\nu}\right].
\end{aligned}$$

The denominator can be decomposed as

$$\frac{1}{\epsilon_{\mu\nu}\pm\Omega} = \frac{1}{\varepsilon_{\mu\nu}}\left(1\mp\frac{\Omega}{\varepsilon_{\mu\nu}\pm\Omega}\right), \qquad (124)$$

where $\varepsilon_{\mu\nu} \equiv \varepsilon_\mu - \varepsilon_\nu$. Substitute this to Eq. (123), then the first term of the decomposition would cancel with the diamagnetic term, because of the following f-sum rule:

$$\frac{1}{V_0}\sum_{\mu\nu}(f_\mu-f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\varepsilon_{\mu\nu}} = -m\rho_0\delta_{\alpha\beta}. \qquad (125)$$

As a result,

$$\sigma_{\alpha\beta}(0,\omega) = \frac{e^2}{im^2V_0}\sum_{\mu\nu}(f_\mu-f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\varepsilon_{\mu\nu}(\Omega+\varepsilon_{\mu\nu})}. \qquad (126)$$

Let's apply this to a metal, and consider only the intra-band contribution, such that $|\mu\rangle,|\nu\rangle$ are the Bloch states $|n\mathbf{k}\rangle,|n\mathbf{k}'\rangle$ (see p. 414 of Ref. 6). For small q, but before taking $q = 0$, we have

$$\langle n\mathbf{k}'|e^{i\mathbf{q}\cdot\mathbf{r}}p_\beta|n\mathbf{k}\rangle \simeq mv_\beta\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}}. \qquad (127)$$

Thus,

$$\sigma_{\alpha\beta}(\mathbf{q},\omega) \simeq \frac{2e^2}{iV_0}\sum_k\frac{f_k-f_{k+q}}{\omega_k-\omega_{k+q}}\frac{v_\alpha v_\beta}{\omega_k-\omega_{k+q}+\omega+i\delta}. \qquad (128)$$

For $q \ll k$, we have

$$\frac{f_{k+q}-f_k}{\omega_{k+q}-\omega_k} \simeq \frac{\partial f}{\partial\varepsilon}. \qquad (129)$$

It follows that,

$$\begin{aligned}
&\sigma_{\alpha\beta}(\mathbf{q},\omega) \\
&\simeq 2ie^2\int\frac{d^3k}{(2\pi)^3}\left(-\frac{\partial f}{\partial\varepsilon}\right)\frac{v_\alpha v_\beta}{\omega_k-\omega_{k+q}+\omega+i\delta} \\
&= 2e^2\int\frac{d^3k}{(2\pi)^3}\left(-\frac{\partial f}{\partial\varepsilon}\right)\frac{v_\alpha v_\beta\tau}{1-i\tau(\omega-\mathbf{q}\cdot\mathbf{v})}, \qquad (130)
\end{aligned}$$

in which we have used $\omega_k - \omega_{k+q} \simeq -\mathbf{q}\cdot\mathbf{v}$, and the relaxation time $\tau = 1/\delta$. This agrees with the result based on the Boltzmann equation (e.g., see Sec. 23.2 of Marder's).

Finally, in the uniform limit,

$$\sigma_{\alpha\beta}(0,\omega) = \frac{2ie^2}{\omega+i\tau^{-1}}\int\frac{d^3k}{(2\pi)^3}\left(-\frac{\partial f}{\partial\varepsilon}\right)v_\alpha v_\beta. \qquad (131)$$

When $\omega\tau \gg 1$, the real part of the conductivity approaches a Dirac delta function. Define a broadened delta function as,

$$\delta_\tau(\omega) = \frac{1}{\pi}\frac{\tau}{1+(\omega\tau)^2}, \qquad (132)$$

then,

$$\text{Re }\sigma_{\alpha\beta}(0,\omega) = D\ \delta_\tau(\omega) + \text{Re }\sigma^{Reg}_{\alpha\beta}(0,\omega). \qquad (133)$$

The coefficient D is known as as the **Drude weight** (see Fig. 4). We have added a possible regular part at higher frequency due to inter-band transition.

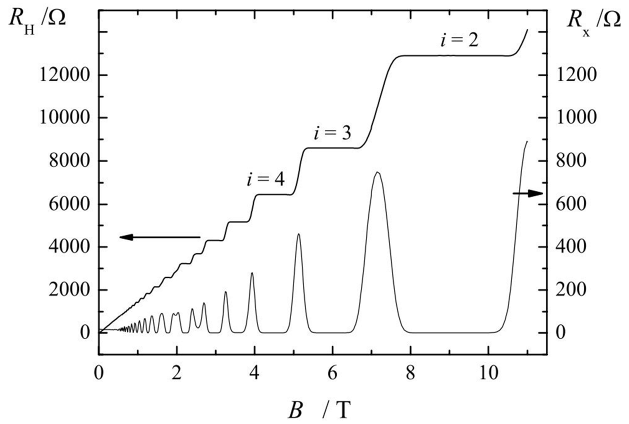

FIG. 5 Quantized Hall conductivity of a 2D electron gas in strong magnetic field.

Remark: For the longitudinal conductivity, in general,

$$\lim_{q\to 0}\lim_{\omega\to 0}\sigma_{\alpha\alpha}(\mathbf{q},\omega)\neq\lim_{\omega\to 0}\lim_{q\to 0}\sigma_{\alpha\alpha}(\mathbf{q},\omega). \tag{134}$$

To get the correct DC conductivity, one needs to take the limit on the RHS. For the limit on the left, the energy levels are discrete while the system is still finite (finite q). As a result, inter-level transitions would be frozen in the DC limit ($\omega\to 0$), and the current vanishes.

2. Hall conductivity, uniform and static

Finally, we would like to consider the DC Hall conductivity. According to Eq. (126), it can be re-written as

$$\sigma^{DC}_{\alpha\neq\beta}=\frac{e^2}{iV_0}\sum_{\mu\nu,\mu\neq\nu}f_\mu\frac{\langle\mu|v_\alpha|\nu\rangle\langle\nu|v_\beta|\mu\rangle-\langle\mu|v_\beta|\nu\rangle\langle\nu|v_\alpha|\mu\rangle}{\varepsilon^2_{\mu\nu}}. \tag{135}$$

If the single-particle states are Bloch states ($\mu\to n\mathbf{k}$), $\langle\mathbf{r}|n\mathbf{k}\rangle=e^{i\mathbf{k}\cdot\mathbf{r}}u_{nk}(\mathbf{r})$, where $u_{nk}(\mathbf{r})$ is the cell-periodic function. Define $\tilde{H}_\mathbf{k}\equiv e^{-i\mathbf{k}\cdot\mathbf{r}}H(\mathbf{r},\mathbf{p})e^{i\mathbf{k}\cdot\mathbf{r}}$, then

$$\begin{aligned}\langle n\mathbf{k}|\frac{\mathbf{p}}{m}|n'\mathbf{k}\rangle &= \langle u_{n\mathbf{k}}|\frac{\mathbf{p}+\hbar\mathbf{k}}{m}|u_{n'\mathbf{k}}\rangle\\ &= \langle u_{n\mathbf{k}}|\frac{\partial\tilde{H}_\mathbf{k}}{\hbar\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle.\end{aligned} \tag{136}$$

With the help of the identity (for $\mu\neq\nu$),

$$\langle u_{n\mathbf{k}}|\frac{\partial\tilde{H}_\mathbf{k}}{\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle=(\varepsilon_{n\mathbf{k}}-\varepsilon_{n'\mathbf{k}})\langle\frac{\partial u_{n\mathbf{k}}}{\partial\mathbf{k}}|u_{n'\mathbf{k}}\rangle, \tag{137}$$

one can show that,

$$\sigma^{DC}_{\alpha\neq\beta}=\frac{e^2}{\hbar V_0}\sum_{nk}f_{nk}\underbrace{\frac{1}{i}\left(\left\langle\frac{\partial u_{nk}}{\partial k_\alpha}|\frac{\partial u_{nk}}{\partial k_\beta}\right\rangle-\left\langle\frac{\partial u_{nk}}{\partial k_\beta}|\frac{\partial u_{nk}}{\partial k_\alpha}\right\rangle\right)}_{\text{Berry curvature }\Omega^\gamma_{nk}}, \tag{138}$$

where α,β, and γ are cyclic. This is also known as the **TKNN formula** (see Ref. 7).

In 2D, for a filled band (usually a Landau subband),

$$C_1^{(n)}\equiv\frac{1}{2\pi}\int_{\text{filled BZ}}d^2k\,\Omega^z_{nk} \tag{139}$$

must be an integer (see Sec. II.B of Ref. 8). Therefore, the Hall conductivity from filled bands is quantized,

$$\sigma^{DC}_{xy}=\frac{e^2}{h}\sum_{\text{filled }n}C_1^{(n)}. \tag{140}$$

The quantized (topological) nature of such an integral is first shown by D.J. Thouless to explain the **integer quantum Hall effect** (see Fig. 5). Note that $h/e^2\simeq 25.813$ kΩ, and quantized Hall resistance $R_H=\frac{h}{e^2}/i$, where i is a positive integer.

1. (a) Show that the Fourier transformations of the Coulomb potential $\phi(r)=1/r$ in 3D and 2D are,

$$\text{3D}:\ \phi(q)=\frac{4\pi}{q^2};\quad \text{2D}:\ \phi(q)=\frac{2\pi}{q}. \tag{141}$$

(b) Show that the density of states of free electron gases in 3D and 2D are,

$$\text{3D}:\ D(\varepsilon_F)=\frac{mk_F}{\pi^2\hbar^2};\quad \text{2D}:\ D(\varepsilon_F)=\frac{m}{\pi\hbar^2}. \tag{142}$$

2. Put a point charge Q in a 2D electron gas.
(a) Under the long-wavelength (Thomas-Fermi) approximation (i.e., $\chi_\rho(\mathbf{q})=-m/\pi\hbar^2$ in Eq. (75) is used), show that the screened electrostatic potential at $k_Fr\gg 1$ is,

$$\phi(\mathbf{r})=\frac{Q}{r}-Q\frac{\pi q_0}{2}[\mathbf{H}_0(q_0r)-N_0(q_0r)], \tag{143}$$

where $q_0=4\pi me^2/h$, $\mathbf{H}_0(x)$ is a Struve function, and $N_0(x)$ is a von Neumann function. Related integral can be found in, for example, Gradshteyn and Ryzhik's *Table of integrals, series, and products.*
(b) Following (a), show that at large distance,

$$\phi(\mathbf{r})\simeq\frac{Q}{q_0^2r^3}. \tag{144}$$

Note: If the complete form of Eq. (75) is used, then

$$\phi(\mathbf{r})\simeq Q\frac{\sin(2k_Fr)}{(2k_Fr)^2}, \tag{145}$$

which shows the Friedel oscillation. Ref: Frank Stern, Phys. Rev. Lett. **18**, 546 (1967). Also, p. 225 of Ref. 1.
3. Assume $H_0=p^2/2m+V_L(\mathbf{r})$. With the help of

$$[H_0,r_\alpha]=\frac{\hbar}{im}p_\alpha, \tag{146}$$

derive the f-sum rule,

$$\frac{1}{V_0}\sum_{\mu\nu}(f_\mu - f_\nu)\frac{\langle\mu|p_\alpha|\nu\rangle\langle\nu|p_\beta|\mu\rangle}{\varepsilon_{\mu\nu}} = -m\rho_0\delta_{\alpha\beta}, \quad (147)$$

in which ρ_0 is the particle density.

4. Start from Eq. (126), derive the conductivity sum rule,

$$\int_{-\infty}^{\infty}\text{Re }\sigma_{\alpha\alpha}(\omega)d\omega = \frac{1}{4}\omega_p^2. \quad (148)$$

That is, the area below a curve in Fig. 4 is fixed by the plasmon frequency. More sum rules can be found in, e.g., Chap 4 of Pines and Nozières, *The theory of quantum liquids*, Addison-Wesley Publishing, 1989.

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