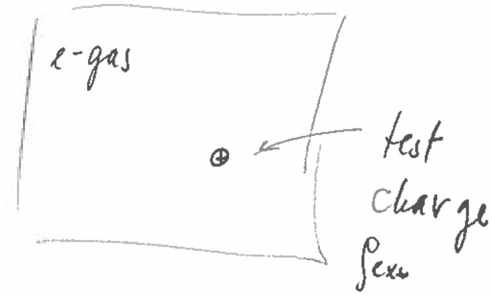
LECTURE 13

Dielectric response of a dense electron gas, screening.

- consider interacting electron gas weakly perturbed by "external" charge density



$$H_{tot} = H + H_{ext}$$

H: e gas with Coulomb interaction

$$H_{ext} = \int d^3x \int d^3x' \, \rho(\vec{x}) \, V(\vec{x} - \vec{x}') \, \rho_{ext}(\vec{x}')$$

- Introduce the dielectric response function $\varepsilon(\vec{q}, \omega)$ by

$$\left[\langle \rho_{tot}(\vec{q}, \omega) \rangle = \rho_{ext}(\vec{q}, \omega) + \langle \rho_{ind}(\vec{q}, \omega) \rangle = \frac{\rho_{ext}(\vec{q}, \omega)}{\varepsilon(\vec{q}, \omega)} \right]$$

- Note:
  - this is the same diel. "constant" as in E & M theory $\vec{D} = \varepsilon \vec{E}$, see p. 142 in D & S.
  - Definition above focuses attention to zeroes

    $\boxed{\varepsilon(\vec{q}, \omega) = 0}$ when arbitrarily weak perturbation gives large response

    this equation defines "free oscillation modes" of the e-gas.

• We calculate $\varepsilon(\vec{q},\omega)$ using linear response theory.

$$\langle \rho_{ind}(\vec{x},t)\rangle = \langle E(t)|\rho(\vec{x})|E(t)\rangle$$

state of the system at time t that has evolved from ground state $|E\rangle$ of H under H_{tot}.

- proceed exactly as in derivation of conductivity:

$$\langle \rho_{ind}(\vec{x},t)\rangle = i\int_0^t dt' \langle [H_{ext}(t'), \rho(\vec{x},t)]\rangle$$

$$= \int_{-\infty}^{\infty} dt' \int d^3x' \int d^3x'' \, \mathcal{K}(\vec{x}-\vec{x}'; t-t') \, V(\vec{x}'-\vec{x}'') \, \rho_{ext}(\vec{x}'',t')$$

where

$$\mathcal{K}(\vec{x}-\vec{x}'; t-t') = -i\theta(t-t')\langle[\rho(\vec{x},t), \rho(\vec{x}',t')]\rangle$$

Kubo formula for dielectric susceptibility

• Simpler structure in momentum/freq. space:

$$\langle \rho_{ind}(\vec{q},\omega)\rangle = V(\vec{q})\,\mathcal{K}(\vec{q},\omega)\,\rho_{ext}(\vec{q},\omega)$$

$$\mathcal{K}(\vec{q},\omega) = -i\int dt \, e^{i\omega t}\,\theta(t)\,\langle[\rho(\vec{q},t), \rho(-\vec{q},0)]\rangle$$

$$\rho(\vec{q}) = \sum_p c^\dagger_{p+q} c_p \quad \leftarrow \text{density operator}$$

It follows that

$$\boxed{\frac{1}{\varepsilon(\vec{q},\omega)} = 1 + V(\vec{q})\, \mathcal{K}(\vec{q},\omega)}$$

<u>The particle-hole GF and the random phase approximation.</u>

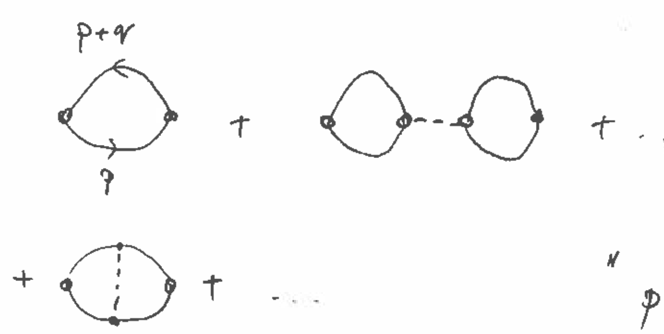
As before we consider time-ordered version

$$\mathcal{K}^T(\vec{q},t) = -i \langle T[\rho(\vec{q},t)\,\rho(-\vec{q},0)] \rangle$$

$$= -i \frac{\langle \phi_0 | T[\rho(\vec{q},t)\,\rho(-\vec{q},0)\, S] | \phi_0 \rangle}{\langle \phi_0 | S | \phi_0 \rangle}$$

and calculate this using FD expansion and diagrams in $(\vec{q},\omega)$ space.

$\mathcal{K}^T(\vec{q},\omega) =$



"polarization propagators"

- Introduce <u>irreducible polarization $\mathcal{P}(\vec{q},\omega)$</u> as the sum of all diagrams that cannot be divided by cutting a single DASHED line.

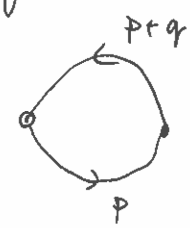
$$\mathcal{K}^T(\vec{q},\omega) = \mathcal{P} + \mathcal{P}V\mathcal{P} + \mathcal{P}V\mathcal{P}V\mathcal{P} + \ldots$$

$$= \mathcal{P} + \mathcal{P}V\left(\mathcal{P} + \mathcal{P}V\mathcal{P} + \ldots\right)$$

$$= \mathcal{P} + \mathcal{P}V\mathcal{K}^T \qquad \leftarrow \text{Dyson's eq. for the particle-hole GF}$$

$$\boxed{\mathcal{K}^T(\vec{q},\omega) = \frac{\mathcal{P}(\vec{q},\omega)}{1 - \mathcal{P}(\vec{q},\omega)\,V(\vec{q})}}$$

The random-phase approximation (RPA) consists of retaining only the leading polarization "buble" diagram

$\mathcal{P}_0(\vec{q},\omega) =$ 

$$= 2(-1)i\int \frac{d^4p}{(2\pi)^4}\, G^0(p+q)\, G^0(p)$$

$$= -2i\int \frac{d^4p}{(2\pi)^4}\, \frac{1}{(p_0+\omega-\varepsilon_{p+q}+i\eta_{p+q})}\, \frac{1}{(p_0-\varepsilon_p+i\eta_p)}$$

$$\eta_p = \begin{cases} 0^+, & |p| > p_F \\ 0^-, & |p| < p_F \end{cases}$$

- Textbook shows evaluation of $\int \frac{dp_0}{(2\pi)} \ldots$ directly at $T=0$ and derivation of $\mathcal{K}(\vec{q},\omega)$ from $\mathcal{K}^T(\vec{q},\omega)$.
- Here we use the result of Probem set 3 (problem 3) where we evaluated $\mathcal{P}(\vec{q},\omega)$ at non-zero T.

$$\mathcal{P}_0(\vec{q}, \omega_n) = \sum_p \frac{f_p - f_{p+q}}{i\omega_n - \varepsilon_p + \varepsilon_{p+q}}$$

Perform analytical continuation $i\omega_n \to \omega + i\varepsilon$ to obtain RETARDED polarization

$$\boxed{\mathcal{P}_0^R(\vec{q}, \omega) = \sum_p \frac{f_p - f_{p+q}}{\omega - \varepsilon_p + \varepsilon_{p+q} + i\varepsilon}}$$

$\varepsilon = 0^+$

coincides with Eq. (6.5.15) D&S

From this we obtain $\mathcal{K}(\vec{q}, \omega)$ directly using Dyson's eq

$$\boxed{\mathcal{K}(\vec{q}, \omega) = \frac{\mathcal{P}_0^R(\vec{q}, \omega)}{1 - \mathcal{P}_0^R(\vec{q}, \omega)\, V(\vec{q})}}$$

and

$$\varepsilon^{-1} = 1 + \mathcal{K} V = 1 + \frac{\mathcal{P}_0^R V}{1 - \mathcal{P}_0^R V} = \frac{1}{1 - \mathcal{P}_0^R V}$$

$$\boxed{\varepsilon(\vec{q}, \omega) = 1 - \mathcal{P}_0^R(\vec{q}, \omega)\, V(\vec{q})}$$

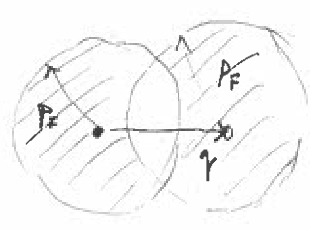
Lindhard dielectric function

A. Static case, $\omega = 0$ $(T=0)$

$$V(\vec{q}) = \frac{4\pi e^2}{q^2} \qquad \varepsilon_p = p^2/2m$$

$$\varepsilon_p - \varepsilon_{p+q} = \frac{1}{2m}\left[p^2 - (\vec{p}+\vec{q})^2\right] = \frac{1}{2m}\left(2\vec{p}\cdot\vec{q} + q^2\right)$$

$$f_p = -\theta(|\vec{p}| - p_F)$$



R

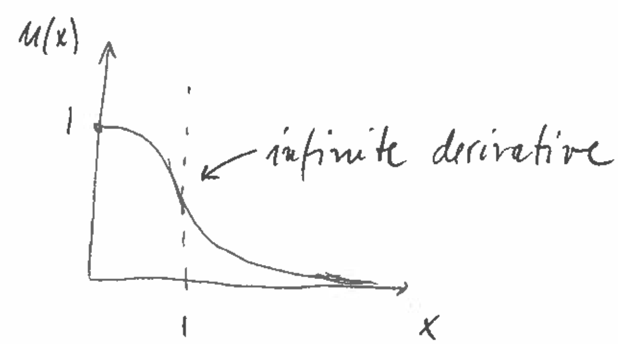
$f_p - f_{p-q}$

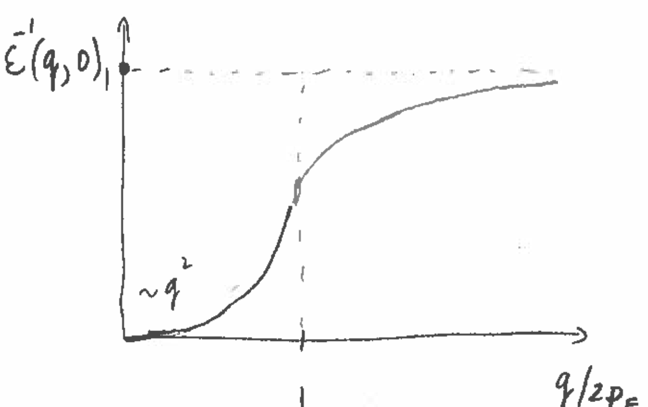
$$\varepsilon(\vec{q},0) = 1 + \frac{4me^2}{\pi^2 q^2}\int_R \frac{d^3p}{2\vec{p}\cdot\vec{q} + q^2}$$

$$= 1 + \frac{4me^2}{\pi q^2}\, u\!\left(\frac{q}{2p_F}\right) = 1 + \left(\frac{4}{9\pi^4}\right)^{1/3} r_s \,\frac{u(x)}{x^2}$$

$$x = q/2p_F, \quad r_s = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{a_0 p_F} \qquad \left(\tfrac{4}{3}\pi (r_s a_0) = V/N\right)$$

$$u(x) = \frac{1}{2}\left\{1 + \frac{1-x^2}{2x}\ln\left|\frac{1+x}{1-x}\right|\right\}$$





• Long wavelength $(q \to 0)$

$u(0) = 1$

$$\varepsilon_{TF}(\vec{q},0) = 1 + \frac{\lambda_{TF}^2}{q^2}, \quad \lambda_{TF}^2 = \frac{4}{\pi} m e^2 p_F$$

↑ Thomas-Fermi diel function

- We can use $\varepsilon(\vec{q},0)$ to define an "effective" or "screened" potential $V_{eff}(\vec{q}) = V(\vec{q})/\varepsilon(\vec{q},0)$. For ε_{TF} we get

$$V_{eff}(\vec{q}) = \frac{4\pi e^2}{q^2\left(1+\frac{\lambda_{TF}^2}{q^2}\right)} = \frac{4\pi e^2}{q^2+\lambda_{TF}^2} \Rightarrow V_{eff}(\vec{r}) \sim \frac{e^{-\lambda_{TF} r}}{r}$$

λ_{TF} - Thomas-Fermi screening length

- The full expression for $\varepsilon(\vec{q},0)$ has sc. length increasing at larger $|\vec{q}|$: electrons become less effective in screening at shorter distances.

- A more careful treatment of full $\varepsilon(\vec{q},0)$ shows that infinite derivative at $|\vec{q}| = 2p_F$ leads to OSCILLATORY behavior of the screened potential at long distances, $V_{eff}(\vec{r}) \sim \frac{\cos(2p_F r)}{r^3}$, "Friedel oscillations" seen in various experiments.

B. Dynamic properties, $\omega \neq 0$ $(T=0)$

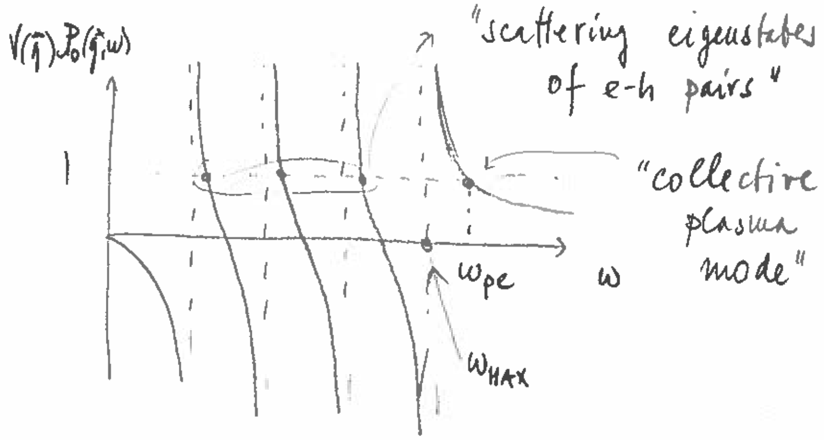
- One can obtain full expression for $\varepsilon(\vec{q},\omega)$ but it is complicated.

- We will analyze physical excitations of the system given by $\varepsilon(\vec{q},\omega) = 0$ or

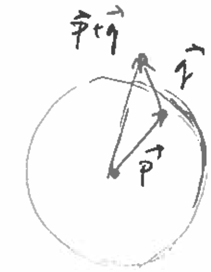
$$V(\vec{q})\,\mathcal{P}_0(\vec{q},\omega) = 1$$

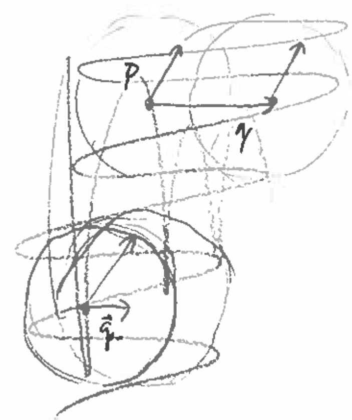
at $T=0$:

$$\mathcal{P}_0(\vec{q},\omega) = \sum_{\substack{p<p_F \\ |\vec{p}+\vec{q}|>p_F}} \left\{ \frac{1}{\omega - \omega_q(p) + i\varepsilon} - \frac{1}{\omega + \omega_q(p) + i\varepsilon} \right\}$$



$$\omega_q(p) \equiv \varepsilon_p - \varepsilon_{p+q}$$





For a fixed $\vec{q}$ ω_{MAX} occurs when $\vec{p} \parallel \vec{q}$ and $|\vec{p}| = p_F$

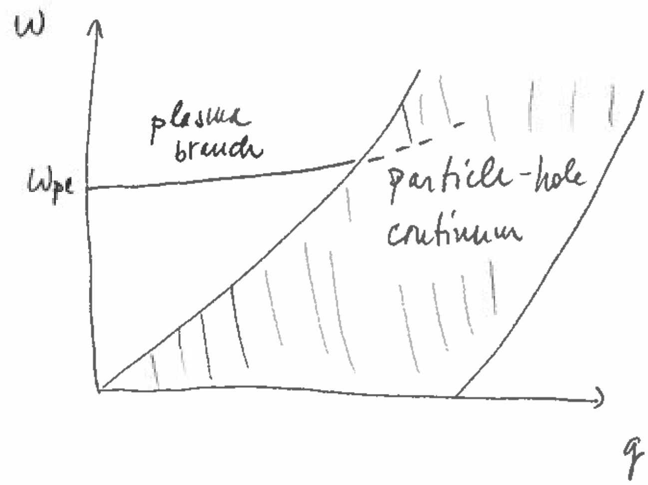
$$\omega_{MAX} = \frac{p_F q}{m} + \frac{q^2}{2m}$$

Crucially, $\omega_{MAX} \to 0$ as $q \to 0$, so in long wavelength limit only the plasma mode survives.

- To find ω_{pe} evaluate $\mathcal{P}_0(\vec{q},\omega)$ as $\vec{q} \to 0$

$$\mathcal{P}_0(\vec{q},\omega) \simeq \sum_{p<p_F} \frac{q^2}{m\omega^2} + O(q^4) = \frac{q^2 N}{m\omega^2} + O(q^4)$$

$$\boxed{\varepsilon(\vec{q},\omega) \simeq 1 - \frac{4\pi N e^2}{m\omega^2} = 1 - \frac{\omega_{pe}^2}{\omega^2}} \qquad \omega_{pe}^2 = \frac{4\pi N e^2}{m}$$


ω
plasma branch
ωpe
particle-hole continuum
q