VIII Training Course in the Physics of
Correlated Electron Systems and High-T_c Superconductors
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Dynamical exchange effects to the dielectric function of a two-dimensional electron gas

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Outline

1. The two-dimensional electron gas: concept & experimental realisations
2. The dielectric function: definition and discussion
3. The dynamical exchange effects: the local field factor
4. Results
    - Dielectric function
    - Plasmon dispersion
    - Structure factor
5. Conclusions

1. The two-dimensional electron gas

A. Concept

- Gas of interacting electrons
- Motion confined in space: restricted to two-dimensions
- Charged particles: undergo Coulomb repulsion
  - $\rightarrow$Neutralising background
- Fermions: obey Pauli-principle
  - $\rightarrow$Importance of exchange effects
- External perturbing field

Model system “jellium”: electrons moving in a homogeneous neutralising background

$\rightarrow$ only one parameter: density of the system

Model Hamiltonian in second quantisation:

$$H = \tfrac{\hbar^2}{2m} \sum_{s} \int d^2 r \nabla y_s^* (\vec{r}) \bullet \nabla y_s (\vec{r})$$

$$+ e \sum_{s} \int d^2 r\, y_s^* (\vec{r}) \Phi^{ext} (\vec{r}, t) y_s (\vec{r})$$

$$+ \tfrac{1}{2} \sum_{s, s'} \int d^2 r \int d^2 r'\, y_s^* (\vec{r}) y_{s'}^* (\vec{r}') v(\vec{r} - \vec{r}', t) y_{s'} (\vec{r}') y_s (\vec{r})$$

with

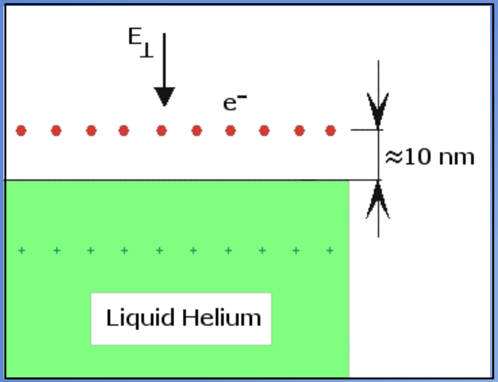
$y_s^* (\vec{r}), y_s (\vec{r})$: the Fermi field operators

$j^{\text{ext}} (\vec{r})$: the external field

$v(\vec{r})$: the Coulomb potential

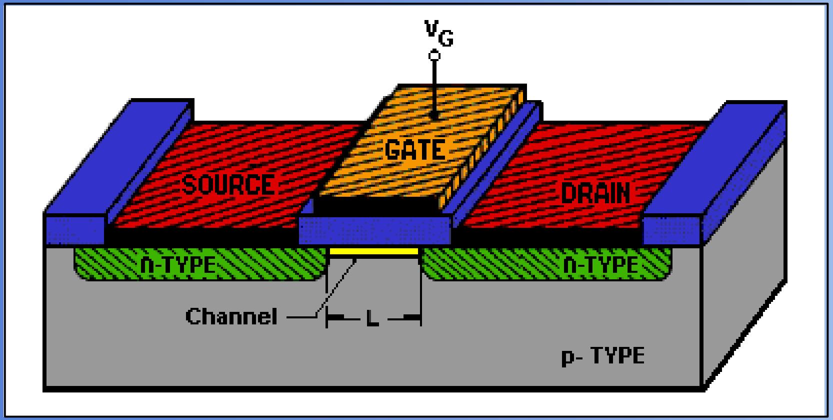
B. Experimental realisations

1) Electrons on the surface of liquid Helium



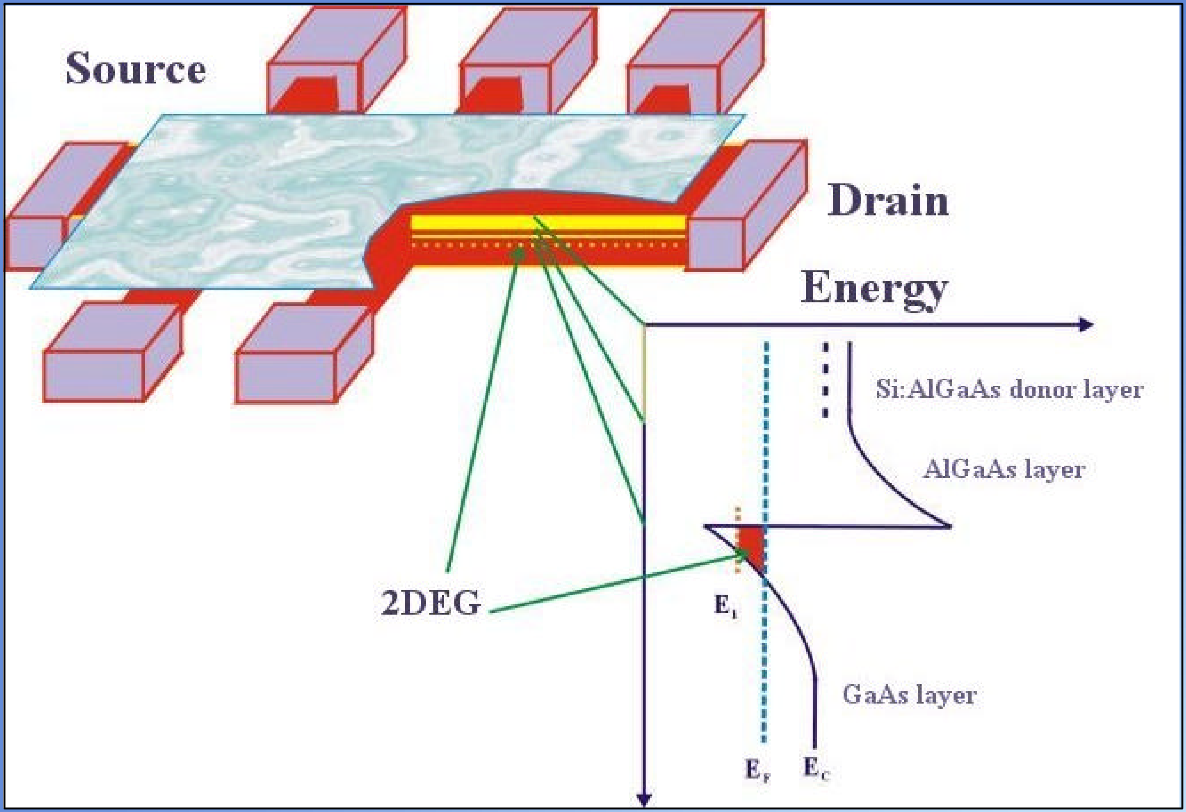
- potential well created in a direction perpendicular to the surface
- nearly ideal 2DES: mobility of the electrons only limited by weak interaction with ripplons
- electron densities limited due to instability of liquid surface

2) Si-MOSFET



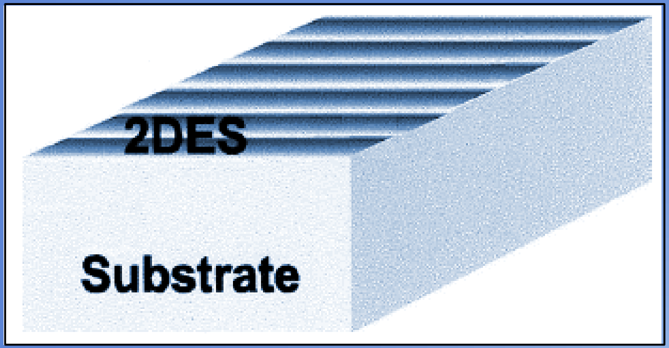
- no current by zero gate voltage
- apply positive gate voltage
- holes in p-type substrate pushed away, electrons attracted
- electrons move in channel below the gate, the inversion layer
- most widely used in industry

3) GaAs-AlGaAs heterostructure



- heterostructure: two semiconductors with nearly same lattice constant, but different band gap
- band bending in the vicinity of the interfaces
- electrons trapped in the confining potential formed at the interface
- very high mobility due to separation of donors and carriers

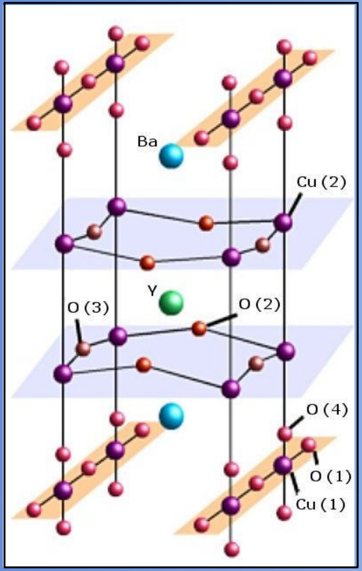
4) Metallic monolayer on substrate



•insulating substrate
•atomic monolayer of metal grown on top
•electrons move freely through toplayer

5) High T_c cuprates

$YBa_2Cu_3O_{7-x}$



•normal phase in overdoped regime
•current running through two-dimensional CuO-planes

2. The dielectric function

A. Definition

$$V_{q,w}^{tc} = \frac{\Phi_{q,w}^{ext}}{e(q,w)}$$

$\Phi_{q,w}^{ext} \rightarrow$ externally applied potential

$V_{q,w}^{tc} \rightarrow$ potential felt by a test charge in the presence of the medium

$$V_{q,w}^{tc} = \Phi_{q,w}^{ext} + v(q) n_{q,w}$$

$n_{q,w} \rightarrow$ induced density in the medium

$v(q) \rightarrow$ Coulomb potential

B. Single particle picture

Free electron gas : electron state $\left|\vec{k}\right\rangle$, energy $E_{\vec{k}} = \dfrac{\hbar^2 k^2}{2m}$

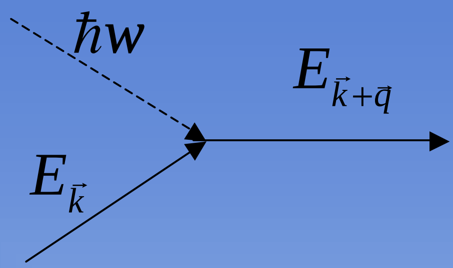
Perturbation $W^{tot}_{q,w}$: total potential felt by the electron

1st order perturbation theory: $\boxed{v(q)n_{q,w} = -Q_0(q,w)W^{tot}_{q,w}}$

Lindhard polarisiblity:

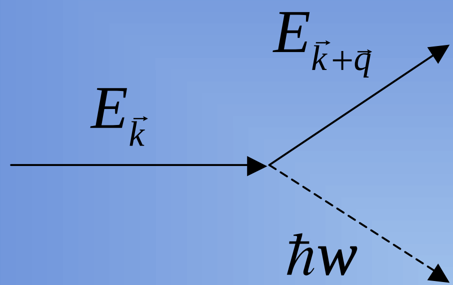
$$Q_0(q,w) = -\frac{2pe^2}{q}\sum_{\left|\vec{k}\right|<k_F}\left(\frac{1}{\hbar w^+ + E_{\vec{k}} - E_{\vec{k}+\vec{q}}} - \frac{1}{\hbar w^+ - E_{\vec{k}} + E_{\vec{k}+\vec{q}}}\right)$$

Absorption:



$$-qk_F + \frac{q^2}{2} \leq \frac{mw}{\hbar} \leq qk_F + \frac{q^2}{2}$$

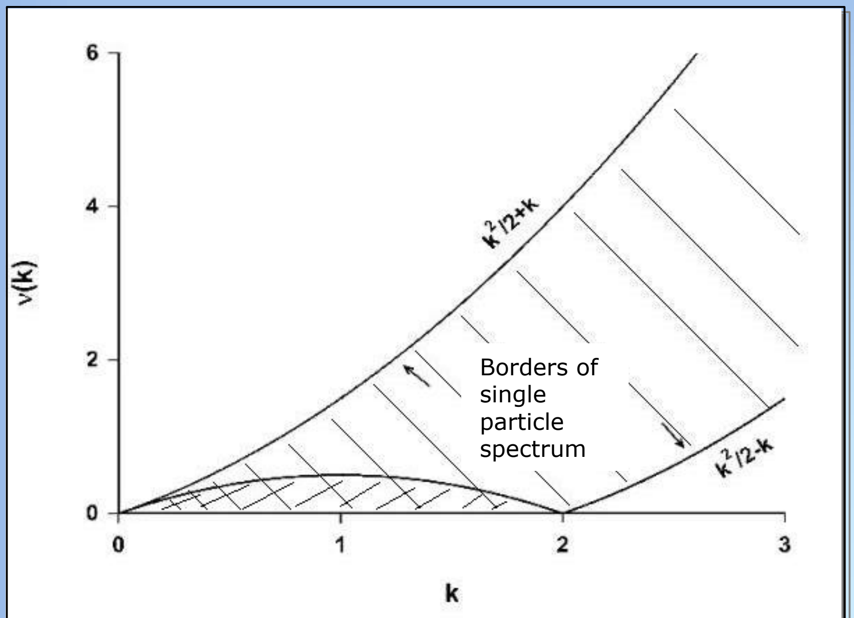
Emission:



$$-qk_F - \frac{q^2}{2} \leq \frac{mw}{\hbar} \leq qk_F - \frac{q^2}{2}$$

- Single particle excitations
- Collective excitations

$\rightarrow$



C. RPA and beyond

Random Phase Approximation:

$$W^{tot}_{q,w} = v(q) n_{q,w} + \Phi^{ext}_{q,w} \qquad \rightarrow \quad e(q,w) = 1 + Q_0(q,w)$$

Exchange and correlation effects

$$W^{tot}_{q,w} = v(q)(1 - G(q,w)) n_{q,w} + \Phi^{ext}_{q,w} \quad \rightarrow \quad e(q,w) = 1 + \frac{Q_0(q,w)}{1 - G(q,w) Q_0(q,w)}$$

$G(q,w)$: local field factor

describes the exchange and correlation hole

3. Dynamical exchange effects

A. Equation of motion

$$i\hbar \frac{d}{dt} n(\vec{r},t) = \left\langle \left[y^{*}(\vec{r}\,') y(\vec{r}), H \right] \right\rangle_t$$

Model Hamiltonian in second quantisation:

$$H = \tfrac{\hbar^2}{2m} \sum_{s} \int d^2 r \nabla y_s^{*}(\vec{r}) \bullet \nabla y_s(\vec{r})$$

$$+ e \sum_{s} \int d^2 r\, y_s^{*}(\vec{r}) \Phi^{ext}(\vec{r},t) y_s(\vec{r})$$

$$+ \tfrac{1}{2} \sum_{s,s'} \int d^2 r \int d^2 r'\, y_s^{*}(\vec{r}) y_{s'}^{*}(\vec{r}\,') v(\vec{r}-\vec{r}\,',t) y_{s'}(\vec{r}\,') y_s(\vec{r})$$

- Hartree-Fock decoupling on the four-field operator terms

$$\left\langle y_1^*(\vec{r}\,')y_2^*(\vec{r}\,')y_3(\vec{r})y_4(\vec{r})\right\rangle$$

$$=\left\langle y_1^*(\vec{r}\,')y_4(\vec{r})\right\rangle\left\langle y_2^*(\vec{r}\,')y_3(\vec{r})\right\rangle-\left\langle y_1^*(\vec{r}\,')y_3(\vec{r})\right\rangle\left\langle y_2^*(\vec{r}\,')y_4(\vec{r})\right\rangle$$

- Linearisation in the external field
- Variational solution of the TDHF-equation

$$\rightarrow e(q,w)=1+\frac{Q_0(q,w)}{1-G(q,w)Q_0(q,w)}$$

B. Local field factor

Expressed in Fermi units, $G(k,n)$ independent of density

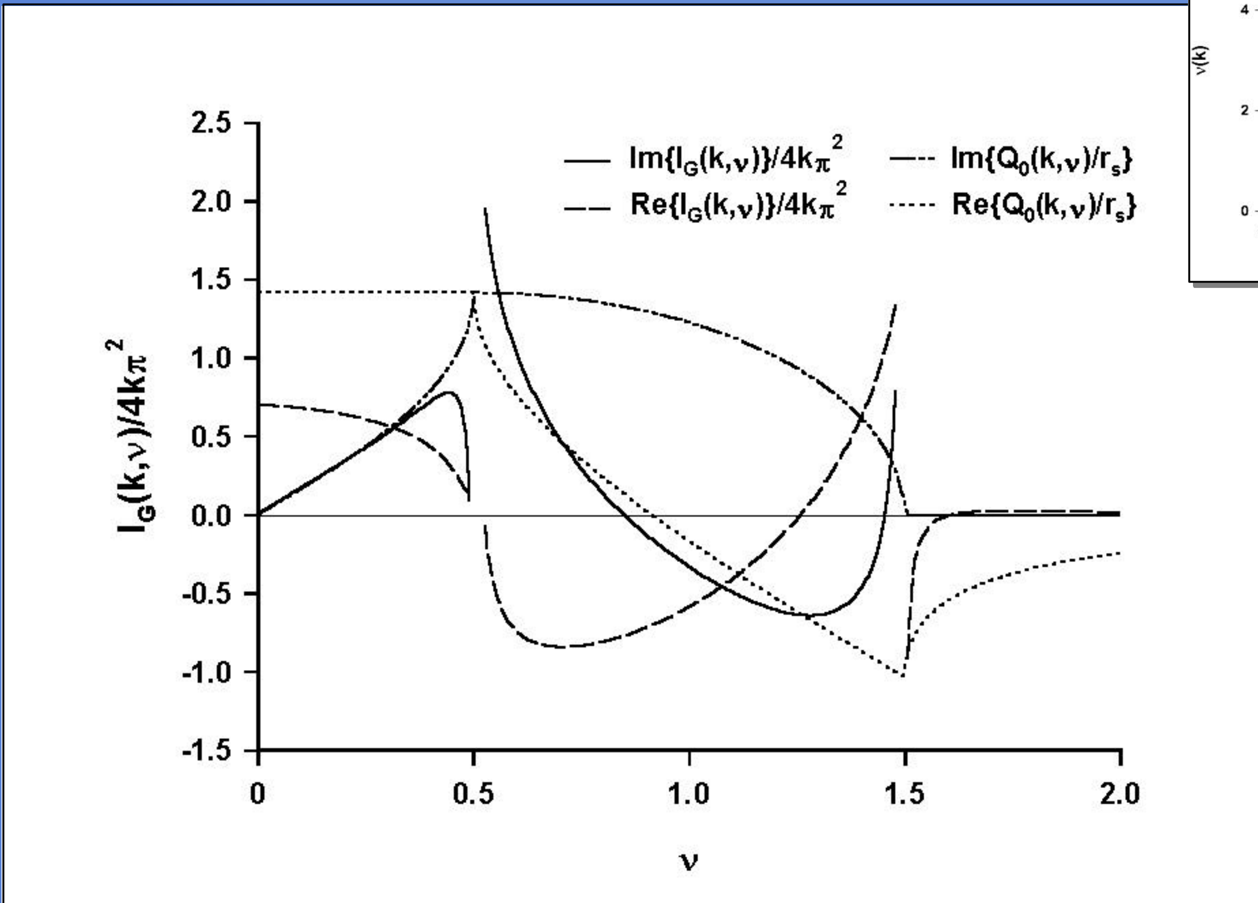
$$G(k,n)=\frac{r_s^2}{4kp^2}\frac{I_G(k,n)}{Q_0^2(k,n)}, \qquad k=\frac{q}{k_F}, \quad n=\frac{\hbar w}{2E_F}.$$

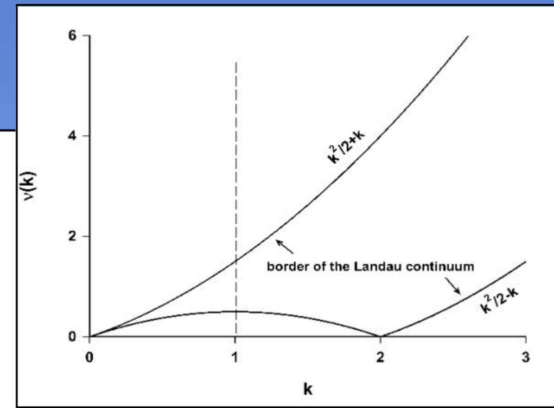
Function $I_G(k,n)$: fourfold integral

$$I_G(k,n)=\int d^2r\int d^2r'\,\frac{\left(N\left(\vec{r}+\frac{\vec{k}}{2}\right)-N\left(\vec{r}-\frac{\vec{k}}{2}\right)\right)\left(N\left(\vec{r}\,'+\frac{\vec{k}}{2}\right)-N\left(\vec{r}\,'-\frac{\vec{k}}{2}\right)\right)}{\left|\vec{r}-\vec{r}\,'\right|}$$

$$\times\frac{1}{n+id-\vec{r}\bullet\vec{k}}\left(\frac{1}{n+id-\vec{r}\,'\bullet\vec{k}}-\frac{1}{n+id-\vec{r}\bullet\vec{k}}\right)$$

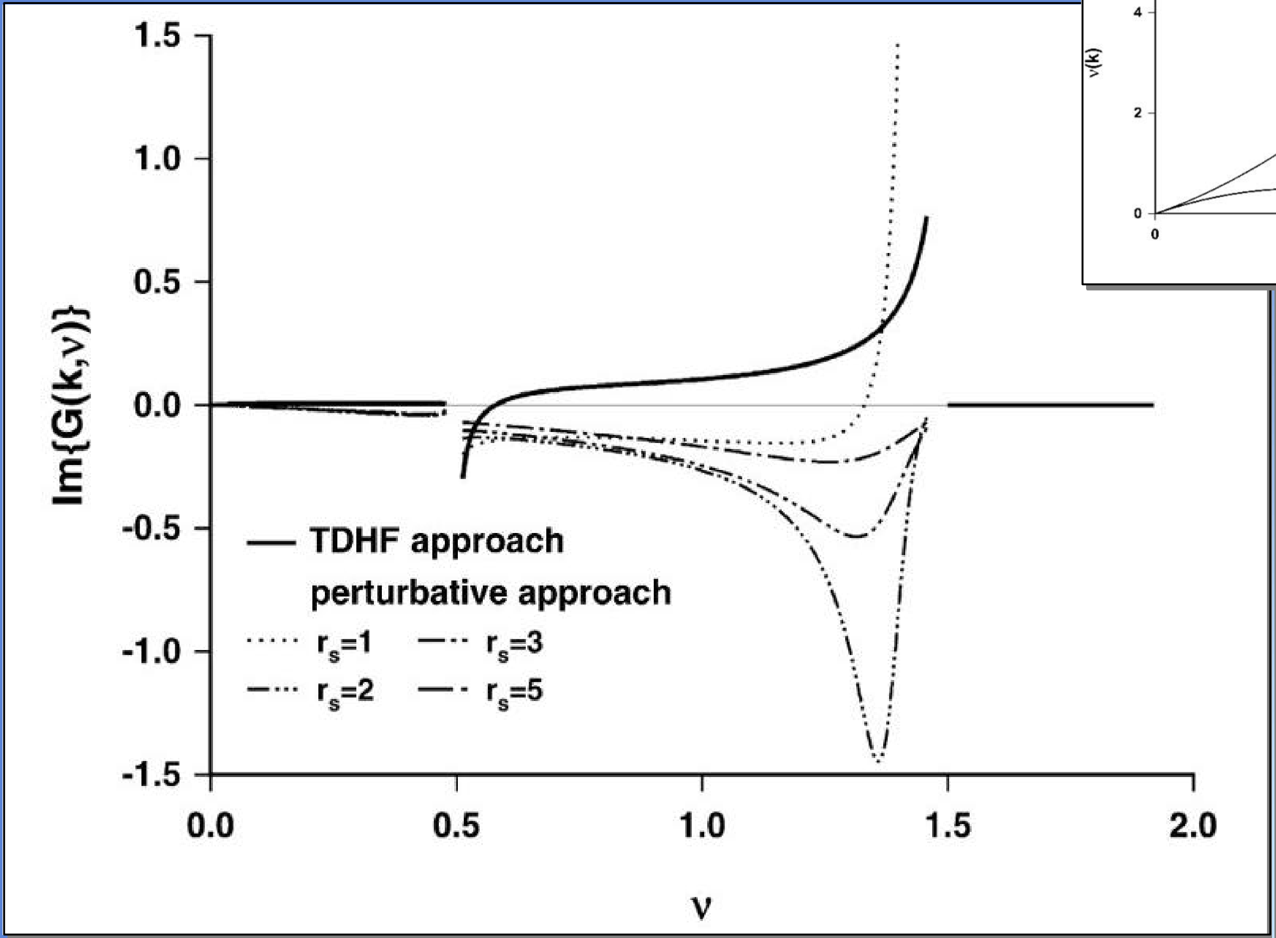
C. Fourfold integral

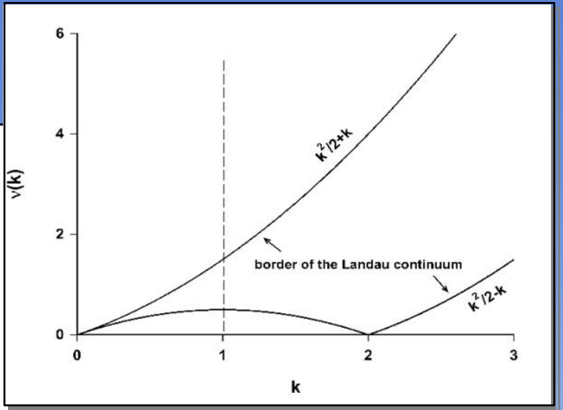




$$G(k,n)=\frac{r_s^2}{4kp^2}\frac{I_G(k,n)}{Q_0^2(k,n)}$$

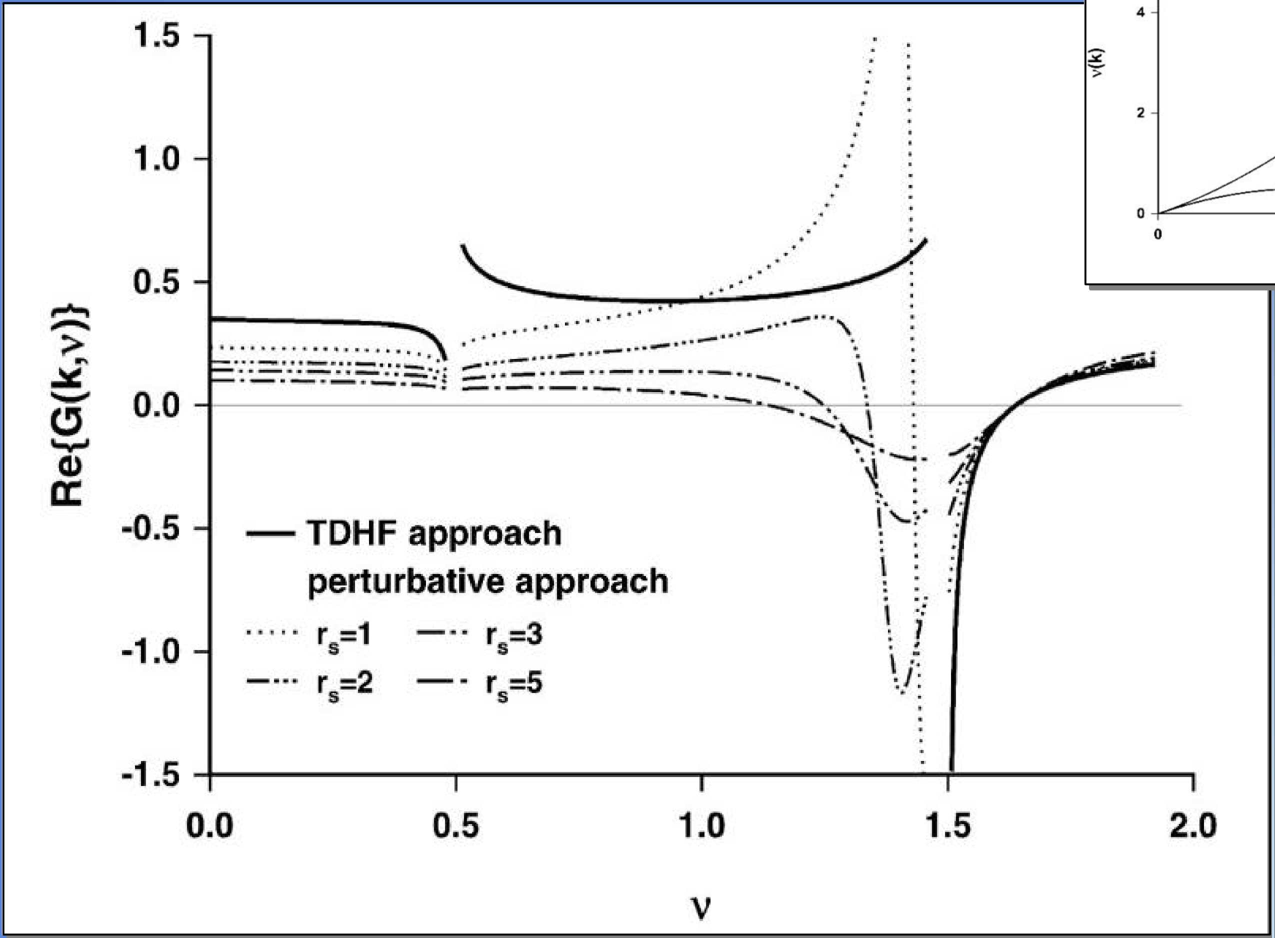
D. Frequency dependence I

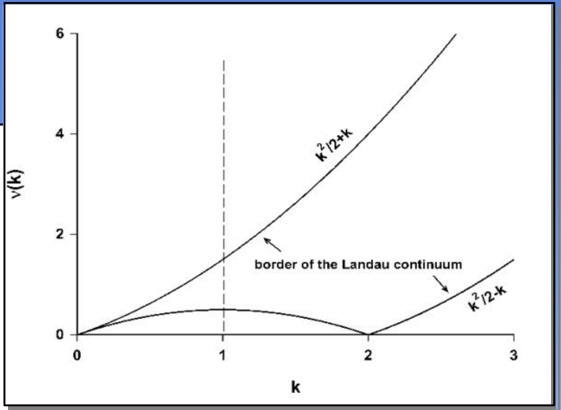




Imaginary part of $G(k,n)$

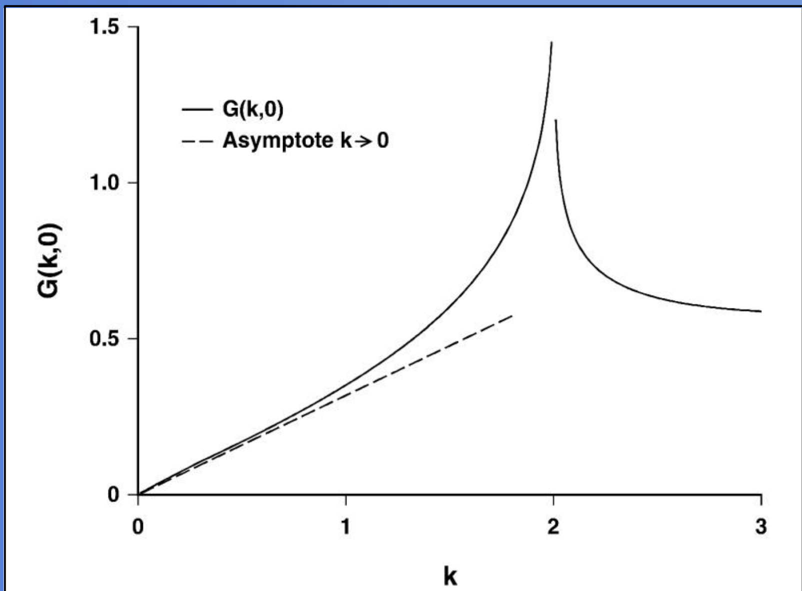
E. Frequency dependence II



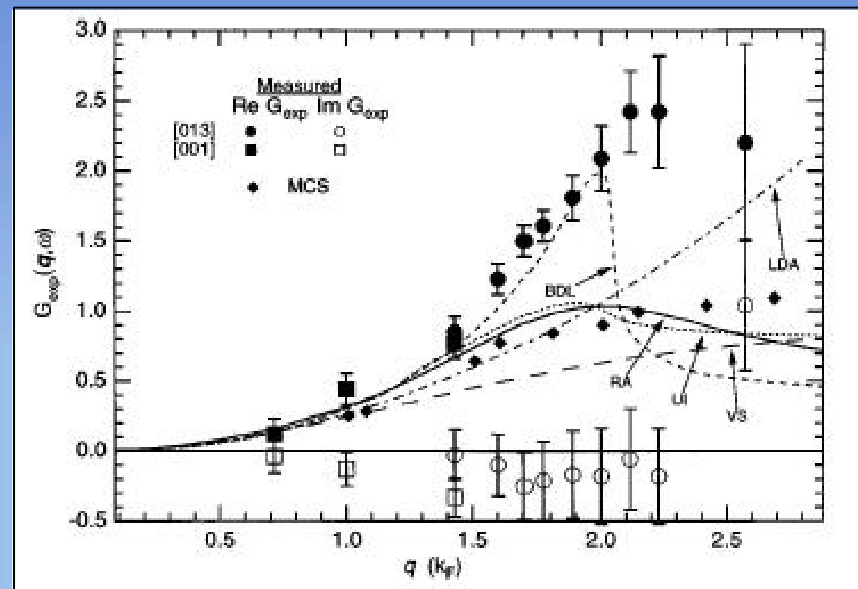


Real part of $G(k,n)$

F. Static case: $G(q,0)$



Static $G(k,0)$



Measured local field factor for Al in 3D

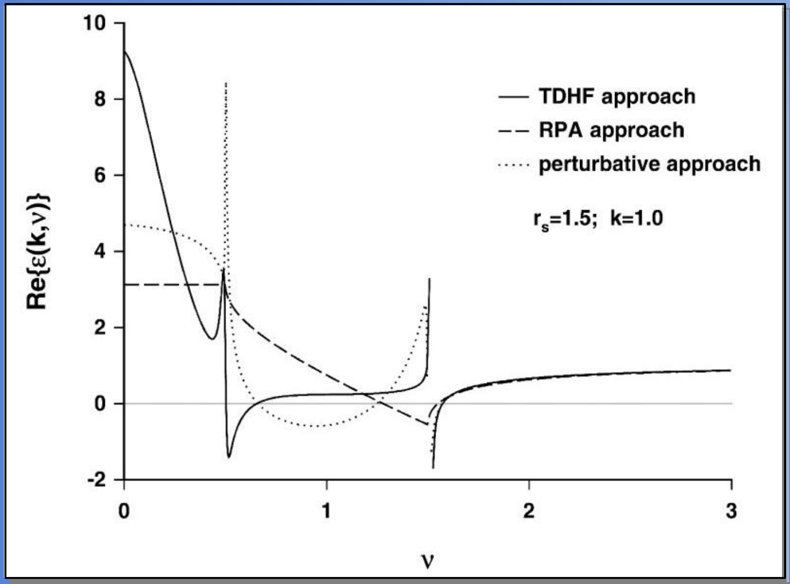
B. C. Larson, J. Z. Tischler, E. D. Isaacs, P. Zschack, A. Fleszar, and A.G. Eguiluz, Phys. Rev. Lett. **77**, 1346 (1996)

4. Results

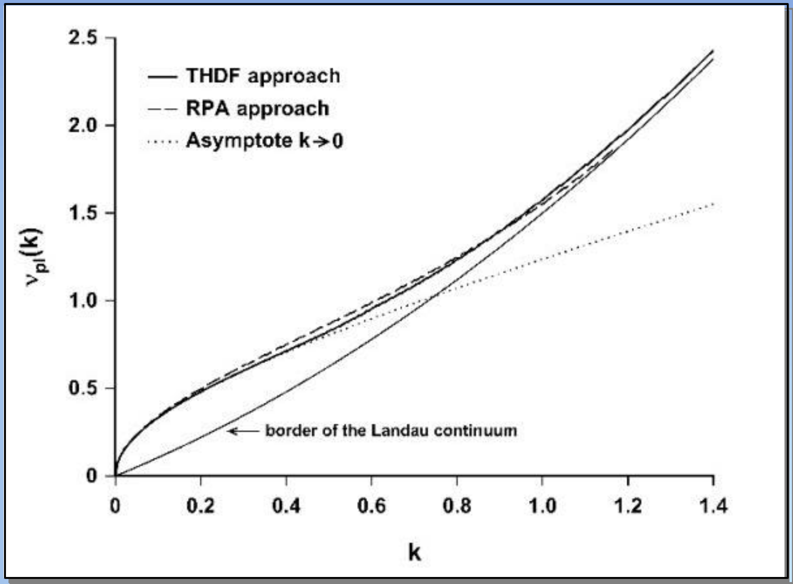
Comparison with:

RPA : $e(q,w) = 1 + Q_0(q,w)$

perturbative approach : $e(q,w) = 1 + Q_0(q,w)\left(1 - G(q,w)Q_0(q,w)\right)$



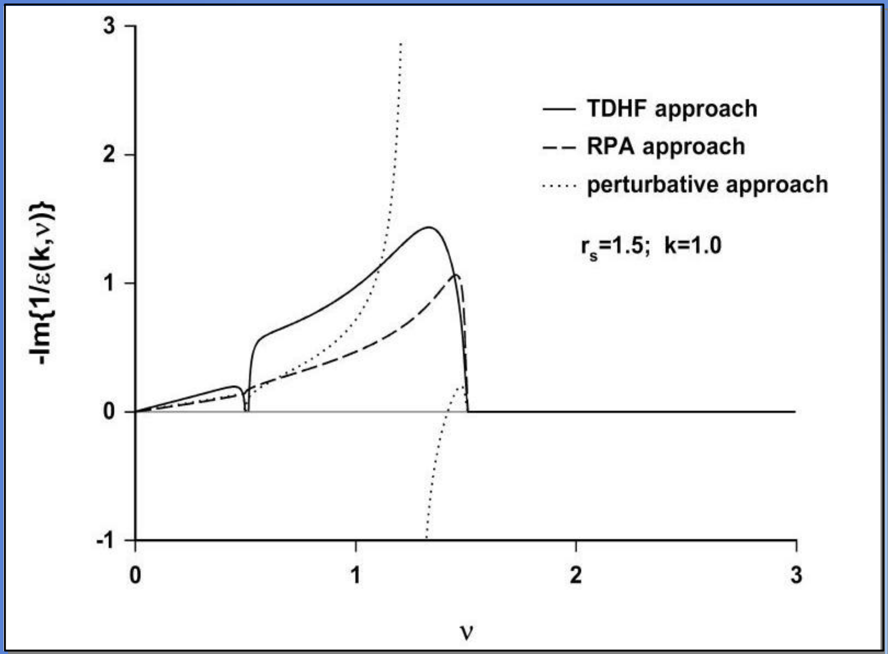
Real part of $e(k,n)$

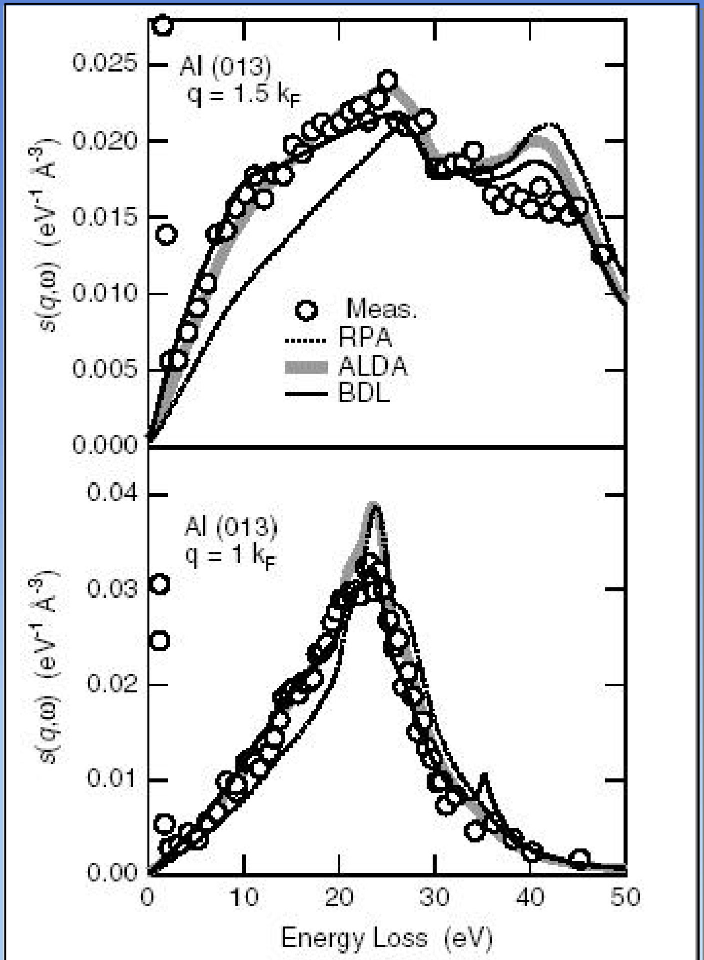


Plasmon dispersion $w_{pl}(k)$

A. Czachor, A. Holas, S. R. Sharma and K. S. Singwi,
Phys. Rev. B **25**, 2144 (1982)

Structure factor





$$S(k,n) \propto \mathrm{Im}\left\{-\frac{1}{e(k,n)}\right\}$$

Absolute IXS-measurements made on Al for $q=k_F$ and $q=1.5k_F$

J. Z. Tischler, B. C. Larson, P. Zschack, A. Fleszar, and A.G. Eguiluz, phys. stat. sol (b) **1**, 280 (2003)

Conclusions

- new expression for the dynamic local field factor $G(k,n)$ of a 2DEG via a variational solution of the TDHF-equation for the density matrix
- $G(k,n)$:
    - takes into account full wave vector and frequency dependence
    - has a pronounced frequency dependence
    - density independent when expressed in Fermi units
    - useful input for DFT
- internal consistency requirements are fulfilled by the current approach; approach extents the perturbative approach of Czachor *et al.*
- inclusion of dynamical exchange effects shown to have a pronounced effect on the dielectric function and the structure factor
- no experiments available yet for the two-dimensional system