CLASE 15 - Martes 18/05/2021

La clase pasada vimos:

Operador densidad de carga

Ecuación de movimiento del operador densidad

Aproximación RPA (Random Phase Approximation)

En esta clase veremos:

En RPA:

Función polarización

Plasmón a q = 0

Contínuo de excitaciones partícula-hueco

REPASO

Operador densidad y operadores de campo

$$\hat{\rho}_e(\mathbf{r}) = -|e|\ \hat{n}(\mathbf{r}) = -|e| \sum_s \hat{\psi}_s^\dagger(\mathbf{r})\hat{\psi}_s(\mathbf{r})$$

$$\hat{\rho}_{e,\mathbf{q}} = -\frac{|e|}{L^3} \sum_{\mathbf{k},s} \hat{a}^\dagger_{\mathbf{k}-\mathbf{q},s}\hat{a}_{\mathbf{k},s}$$

Ecuación de movimiento de Heisenberg (representación de Heisenberg)

REPASO

$$\frac{d}{dt}a^\dagger_{\mathbf{k}-\mathbf{q}}a_{\mathbf{k}} = \frac{i}{\hbar}[\mathcal{H},\, a^\dagger_{\mathbf{k}-\mathbf{q}}a_{\mathbf{k}}]$$

$$\mathcal{H} = \sum_{\mathbf{k}} E_k a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{2}\sum_{\substack{\mathbf{k},\mathbf{k}' \\ \mathbf{q}\neq 0}} V_q a^\dagger_{\mathbf{k}-\mathbf{q}} a^\dagger_{\mathbf{k}'+\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}}$$

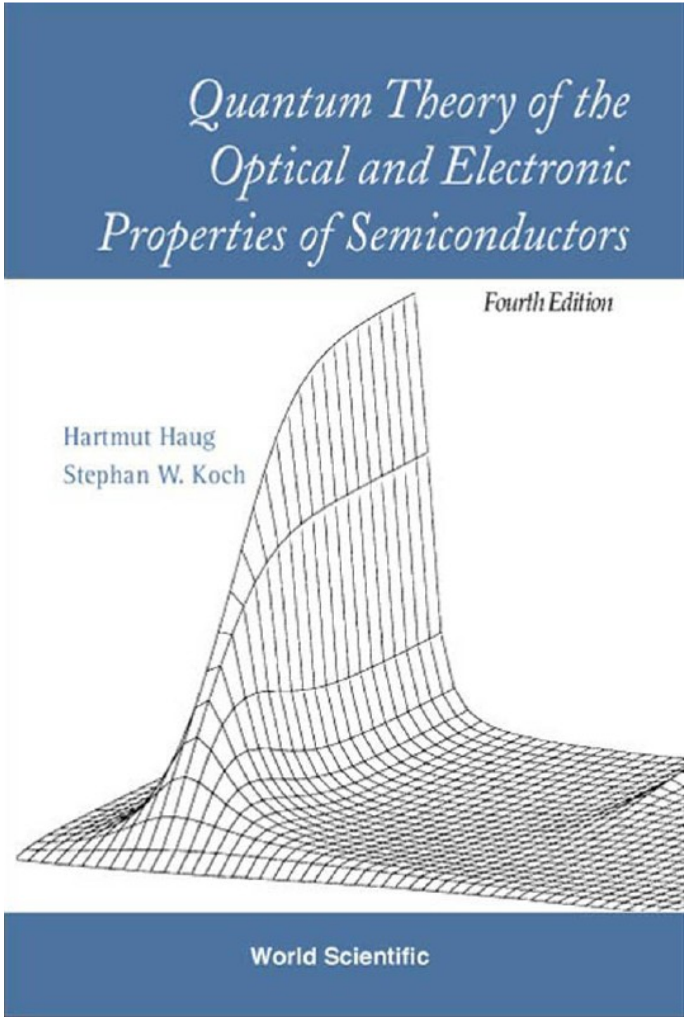
Hamiltoniano del gas de electrones

$$\boxed{\begin{aligned}\frac{d}{dt}\langle a^\dagger_{\mathbf{k}-\mathbf{q}}a_{\mathbf{k}}\rangle &= i(\epsilon_{k-q}-\epsilon_k)\langle a^\dagger_{\mathbf{k}-\mathbf{q}}a_{\mathbf{k}}\rangle \\ &\quad + \frac{i}{\hbar}\sum_{\mathbf{p}',\mathbf{p}} V_p \left(\langle a^\dagger_{\mathbf{k}-\mathbf{q}-\mathbf{p}} a^\dagger_{\mathbf{p}'+\mathbf{p}} a_{\mathbf{p}'} a_{\mathbf{k}}\rangle + \langle a^\dagger_{\mathbf{k}-\mathbf{q}} a^\dagger_{\mathbf{p}'-\mathbf{p}} a_{\mathbf{k}-\mathbf{p}} a_{\mathbf{p}'}\rangle\right)\end{aligned}}$$

$$\frac{d}{dt}\langle a^\dagger_{\mathbf{k}-\mathbf{q}}a_{\mathbf{k}}\rangle \simeq i(\epsilon_{k-q}-\epsilon_k)\langle a^\dagger_{\mathbf{k}-\mathbf{q}}a_{\mathbf{k}}\rangle + \frac{iV_q}{\hbar}(f_{\mathbf{k}}-f_{\mathbf{k}-\mathbf{q}})\sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}}a_{\mathbf{p}'}\rangle$$

RPA

Estamos viendo: plasmones



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Random-phase approximation / Aproximación de fases aleatorias

A hand-waving argument for the random phase approximation is to say that an expectation value $\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} \rangle$ has a dominant time dependence

$$\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} \rangle \propto e^{i(\omega_{\mathbf{k}} - \omega_{\mathbf{k}'})t} \quad . \tag{8.10}$$

These expectation values occur under sums, so that expressions like

$$\sum_{\mathbf{k},\mathbf{k}'} e^{i(\omega_{\mathbf{k}} - \omega_{\mathbf{k}'})t}$$

have to be evaluated. Since terms with $\mathbf{k} \neq \mathbf{k}'$ oscillate rapidly they more or less average to zero, whereas the term with $\mathbf{k} = \mathbf{k}'$ gives the dominant contribution.

Estas serían las fases aleatorias que se cancelan entre sí y se pueden ignorar.

Random-phase approximation (RPA)

$$\frac{d}{dt}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle \simeq i(\epsilon_{k-q} - \epsilon_k)\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle + \frac{iV_q}{\hbar}(f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}})\sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle$$

Hacemos el ansatz : $\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle(t) = e^{-i(\omega+i\delta)t}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle(0)$

$$\Rightarrow \quad \begin{aligned} \frac{d}{dt}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle(t) &= \frac{d}{dt}\left[e^{-i(\omega+i\delta)t}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle(0)\right] \\ &= -i(\omega+i\delta)\, e^{-i(\omega+i\delta)t}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle(0) \\ &= -i(\omega+i\delta)\,\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle(t) \end{aligned}$$

Reemplazando arriba obtenemos:

$$\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle = V_q(f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}})\sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle$$

Random-phase approximation (RPA)

$$\cancel{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}} \rangle = \frac{V_q (f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}) \sum_{\mathbf{p}'} \langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'} \rangle}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}$$

Random-phase approximation (RPA)

$$\cancel{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_\mathbf{k}\rangle = \frac{V_q (f_{\mathbf{k}-\mathbf{q}} - f_\mathbf{k}) \sum_{\mathbf{p}'} \langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}$$

$$\left(\frac{-|e|}{L^3}\right)\sum_\mathbf{k} \langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_\mathbf{k}\rangle = \left(\frac{-|e|}{L^3}\right)\sum_\mathbf{k} \frac{V_q (f_{\mathbf{k}-\mathbf{q}} - f_\mathbf{k})}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} \sum_{\mathbf{p}'} \langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle$$

Random-phase approximation (RPA)

$$\cancel{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle = \frac{V_q(f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}})\sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle}{\hbar(\omega+i\delta+\epsilon_{k-q}-\epsilon_k)}$$

$$\left(\frac{-|e|}{L^3}\right)\sum_{\mathbf{k}} \langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}}\rangle = \left(\frac{-|e|}{L^3}\right)\sum_{\mathbf{k}} \frac{V_q(f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}})}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} \sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle$$

$$= \sum_{\mathbf{k}} \frac{V_q(f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}})}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} \left(\frac{-|e|}{L^3}\right)\sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle$$

Random-phase approximation (RPA)

$$\cancel{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_\mathbf{k}\rangle = \frac{V_q(f_{\mathbf{k}-\mathbf{q}} - f_\mathbf{k})\sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle}{\hbar(\omega+i\delta+\epsilon_{k-q}-\epsilon_k)}$$

$$\underbrace{\left(\frac{-|e|}{L^3}\right)\sum_{\mathbf{k}} \langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_\mathbf{k}\rangle}_{\langle\rho_\mathbf{q}\rangle} = \left(\frac{-|e|}{L^3}\right)\sum_{\mathbf{k}} \frac{V_q(f_{\mathbf{k}-\mathbf{q}} - f_\mathbf{k})}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} \sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle$$

$$= \sum_{\mathbf{k}} \frac{V_q(f_{\mathbf{k}-\mathbf{q}} - f_\mathbf{k})}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} \underbrace{\left(\frac{-|e|}{L^3}\right) \sum_{\mathbf{p}'}\langle a^\dagger_{\mathbf{p}'-\mathbf{q}} a_{\mathbf{p}'}\rangle}_{\langle\rho_\mathbf{q}\rangle}$$

$$\langle\rho_\mathbf{q}\rangle = -\frac{|e|}{L^3}\sum_{\mathbf{k}}\langle a^\dagger_{\mathbf{k}-\mathbf{q}} a_\mathbf{k}\rangle$$

Random-phase approximation (RPA)

$$\langle \rho_{\mathbf{q}} \rangle = V_q \langle \rho_{\mathbf{q}} \rangle \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} \quad \Rightarrow \quad V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)} = 1$$

$$V_q \, P^1(q,\omega) = 1 \quad \Rightarrow \quad P^1(q,\omega) = \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega + i\delta + \epsilon_{k-q} - \epsilon_k)}$$

Función polarización (primer orden)

Con funciones de distribución de equilibrio (Fermi)

$$\delta \to 0 \quad \Rightarrow \quad V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega_q + \epsilon_{k-q} - \epsilon_k)} = 1 \qquad (8.25)$$

Buscamos soluciones de $\omega(q)$ que satisfagan esta ecuación $\rightarrow$ modos normales

Random-phase approximation (RPA)

$$V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega_q + \epsilon_{k-q} - \epsilon_k)} = 1$$

Primero tratemos el caso importante de larga longitud de onda:

$$\left.\begin{array}{l} \lambda \to \infty \\ q \propto 1/\lambda \to 0 \end{array}\right\} \quad \begin{array}{l} E_{k-q} - E_k = \dfrac{\hbar^2}{2m}(k^2 - 2\mathbf{k}\cdot\mathbf{q} + q^2) - \dfrac{\hbar^2 k^2}{2m} \simeq -\dfrac{\hbar^2 \mathbf{k}\cdot\mathbf{q}}{m} \\ f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}} = f_{\mathbf{k}} - \mathbf{q}\cdot\nabla_{\mathbf{k}} f_{\mathbf{k}} + \cdots - f_{\mathbf{k}} \simeq -\mathbf{q}\cdot\nabla_{\mathbf{k}} f_{\mathbf{k}} \end{array}$$

$$\Rightarrow \quad 1 \simeq -V_q \sum_{\mathbf{k},i} \frac{q_i \frac{\partial f}{\partial k_i}}{\hbar\omega_0 - \hbar^2 \mathbf{k}\cdot\mathbf{q}/m}$$

$$\simeq -\frac{V_q}{\hbar\omega_0} \sum_{\mathbf{k},i} q_i \frac{\partial f}{\partial k_i}\left(1 + \frac{\hbar\mathbf{k}\cdot\mathbf{q}}{m\omega_0}\right)$$

Pusimos:

$$\omega_{q\to 0} = \omega_0$$

Random-phase approximation (RPA)

Caso $\lambda \to \infty$

$$1 \simeq -V_q \sum_{\mathbf{k},i} \frac{q_i \frac{\partial f}{\partial k_i}}{\hbar\omega_0 - \hbar^2 \mathbf{k}\cdot\mathbf{q}/m}$$

$$\simeq -\frac{V_q}{\hbar\omega_0} \sum_{\mathbf{k},i} q_i \frac{\partial f}{\partial k_i} \left(1 + \frac{\hbar \mathbf{k}\cdot\mathbf{q}}{m\omega_0}\right)$$

Para el primer término:

$$\sum_{\mathbf{k}} \mathbf{q}\cdot\nabla_{\mathbf{k}} f(\mathbf{k}) = \sum_{\mathbf{k}} \sum_i q_i \frac{\partial f(\mathbf{k})}{\partial k_i}$$

$$= \frac{1}{(\Delta k)^3} \sum_{i=1}^{3} q_i \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \int_{-\infty}^{\infty} dk_z \frac{\partial f(\mathbf{k})}{\partial k_i} = 0$$

$$\Rightarrow \quad 1 = -\frac{V_q}{\hbar\omega_0} \sum_{\mathbf{k},i} q_i \frac{\partial f}{\partial k_i} \frac{\hbar \mathbf{k}\cdot\mathbf{q}}{m\omega_0}$$

Random-phase approximation (RPA)

$$1 = -\frac{V_q}{\hbar\omega_0}\sum_{\mathbf{k},i} q_i \frac{\partial f}{\partial k_i}\frac{\hbar\mathbf{k}\cdot\mathbf{q}}{m\omega_0}$$

Haciendo integración por partes:

$$1 = V_q \frac{q^2}{m\omega_0^2}\sum_{\mathbf{k}} f_{\mathbf{k}} = V_q \frac{q^2 N}{m\omega_0^2} = \frac{4\pi e^2}{\epsilon_0 q^2 L^3}\frac{q^2 N}{m\omega_0^2}$$

$$\omega_0^2 = \frac{4\pi e^2 n}{\epsilon_0 m} = \omega_{pl}^2$$

Recuperamos el resultado obtenido con el modelo de Drude: $q \rightarrow 0\,,\ \omega_{q\rightarrow 0} = \omega_{pl}$

Random-phase approximation (RPA)

Solución para **q** general

$$V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega_q + \epsilon_{k-q} - \epsilon_k)} = V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}}{\hbar} \left(\frac{1}{\omega_q + \epsilon_k - \epsilon_{k+q}} - \frac{1}{\omega_q + \epsilon_{k-q} - \epsilon_k} \right)$$

Hay polos en:

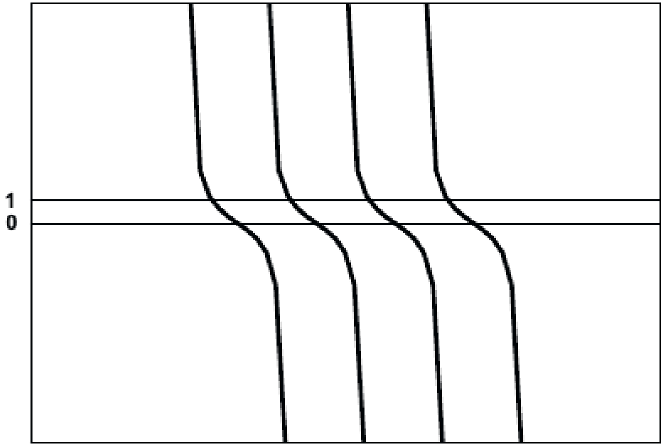
$$\begin{cases} \omega_q = \epsilon_{k+q} - \epsilon_k = \dfrac{\hbar k q}{m} \cos\theta + \dfrac{\hbar q^2}{2m} \\ \omega_q = \epsilon_k - \epsilon_{k-q} = \dfrac{\hbar q k}{m} \cos\theta - \dfrac{\hbar q^2}{2m} \end{cases}$$

$$\theta = \measuredangle(\mathbf{k}, \mathbf{q})$$

Random-phase approximation (RPA)

Solución para **q** general

$$V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega_q + \epsilon_{k-q} - \epsilon_k)} = V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}}{\hbar} \left(\frac{1}{\omega_q + \epsilon_k - \epsilon_{k+q}} - \frac{1}{\omega_q + \epsilon_{k-q} - \epsilon_k} \right)$$



$$V_q \sum_{\mathbf{k}} \frac{f_{\mathbf{k}-\mathbf{q}} - f_{\mathbf{k}}}{\hbar(\omega_q + \epsilon_{k-q} - \epsilon_k)} = 1 \tag{8.25}$$

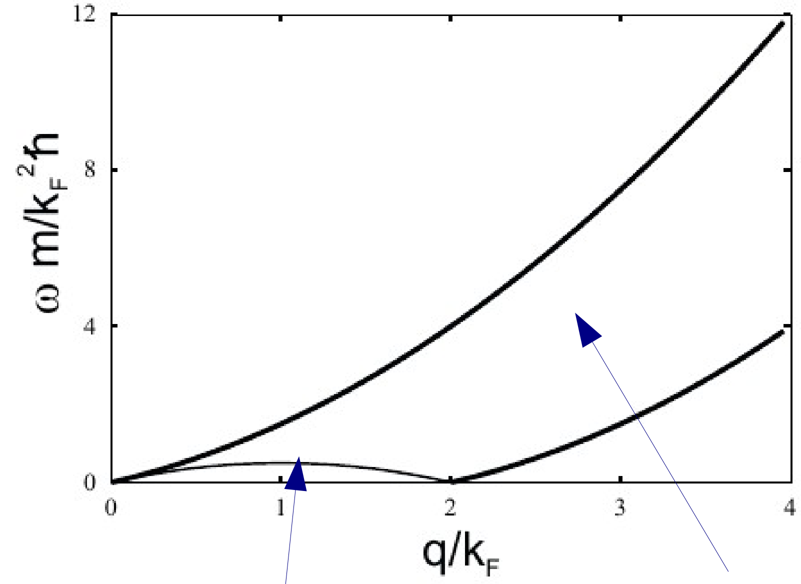
Las soluciones buscadas son los puntos de intersección de la recta en 1 y las curvas. Las soluciones están cerca de los polos.

Fig. 8.1 Graphical solution of Eq. (8.25). The full lines are a schematic drawing of part of the LHS of Eq. (8.25) and the line "1" is the RHS of Eq. (8.25).

Random-phase approximation (RPA)

Análisis a $T \approx 0$

$$\omega_q^{max} = \frac{\hbar q k_F}{m} + \frac{\hbar q^2}{2m}$$



$$\omega_q^{min} = -\frac{\hbar q k_F}{m} + \frac{\hbar q^2}{2m}$$

Fig. 8.2 The thick lines show the boundary of the continuum of pair excitations at $T = 0\,K$, according to Eqs. (8.35) and (8.36), respectively. The thin line is the result of Eq. (8.37).

$$\omega_q^{ext} = \frac{\hbar q k_F}{m} - \frac{\hbar q^2}{2m}$$

Resumen de la clase 15

En RPA:

- Función polarización
- Plasmón a $q = 0$
- Contínuo de excitaciones partícula-hueco